Naval Research Laboratory

Washington, DC 20375-5320

NRL/MR/6390--17-9723

Equilibrium Structures and Absorption Spectra for Si_XO_Y-nH_2O Molecular Clusters using Density Functional Theory

L. Huang
S.G. Lambrakos

Center for Computational Materials Science
Materials Science and Technology Division

L. Massa

Hunter College, City University of New York
New York, New York

May 4, 2017

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
04-05-2017	NRL Memorandum Report	

4. TITLE AND SUBTITLE

Equilibrium Structures and Absorption Spectra for Si_xO_y-nH_2O Molecular Clusters using Density Functional Theory

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

L. Huang, S.G. Lambrakos, and L. Massa[1]

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER
63-4995-07

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Naval Research Laboratory, Code 6394
4555 Overlook Avenue, SW
Washington, DC 20375-5320

8. PERFORMING ORGANIZATION REPORT NUMBER

NRL/MR/6390--17-9723

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Office of Naval Research
One Liberty Center
875 North Randolph Street, Suite 1425
Arlington, VA 22203-1995

10. SPONSOR / MONITOR'S ACRONYM(S)
ONR

11. SPONSOR / MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

[1]Hunter College, City University of New York, New York, NY 10065

14. ABSTRACT

Calculations are presented of vibrational and electronic excited-state absorption spectra for eqilibrium structures of Si_xO_y-nH_2O molecular clusters using density function theory (DFT) and time-dependent density functional theory (TD-DFT). The size of the clusters considered is relatively large compared to those considered in previous studies. DFT and TD-DFT can provide interpretation of absorption spectra with respect to molecular structure for excitation by electromagnetic waves at frequencies within the IR and UV-visible ranges. The absorption spectrum corresponding to excitation states of Si_xO_y-nH_2O molecular clusters consisting of relatively small numbers of atoms should be associated with response features that are intermediate between that of isolated molecules and that of a bulk system. DFT and TD-DFT calculated absorption spectra represent quantitative estimates that can be correlated with additional information obtained from laboratory measurements. The DFT software GAUSSIAN was used for the calculations of excitation states presented here.

15. SUBJECT TERMS

Absorption spectra
Molecular clusters
Density Functional Theory

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
					Samuel G. Lambrakos
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	Unclassified Unlimited	55	**19b. TELEPHONE NUMBER** *(include area code)*
Unclassified Unlimited	Unclassified Unlimited	Unclassified Unlimited			(202) 767-2601

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

Contents

Introduction

Understanding the nature of silicon oxide clusters is of major importance to nanoscience and technology. This follows in that silicon oxide clusters are characterized by many different geometries, which potentially can be optimized with respect to specific materials design criteria, i.e., molecular structures and properties, for systems consisting of nano-scale molecular clusters. Previous studies [1-9] have investigated structures and properties of small to medium-sized Si_xO_y molecular clusters. The present study presents further investigation of structures and properties of medium-sized Si_xO_y-nH_2O molecular clusters using density functional theory (DFT). The size of the clusters considered, however, is relatively large compared to those considered in previous studies.

Density functional theory (DFT) is applied to determine equilibrium structures and absorption spectra for Si_xO_y-nH_2O molecular clusters. DFT applied for the determination of equilibrium molecular structures and absorption spectra provides information complementary to that of experimental results, e.g., reference [10]. Significantly, DFT calculation of absorption spectra can adopt the perspective of computational physics, which is that numerical simulations may be viewed as "experimental`` data. Here DFT calculations of vibrational modes are associated with different molecular structures. DFT is used for calculation of ground state resonance structure to enable physical interpretation of absorption spectra associated with molecular structures excited by IR electromagnetic waves. Such spectra are attributed to optically active vibrational modes. In these studies the DFT calculations were implemented using the computer program GAUSSIAN09 (G09) [11]. The present study also considers calculation of approximate UV-Vis absorption spectra for Si_xO_y-nH_2O molecular clusters, which uses time-dependent density functional theory (TD-DFT) as implemented in GAUSSIAN [11].

This report is organized as follows. First, a general review of vibrational analysis needed for calculation of absorption spectra is presented. Second, DFT calculations of equilibrium energies for Si_xO_y-nH_2O molecular structures are presented. Third, DFT calculations are presented of vibration resonance structure of the Si_xO_y-nH_2O structures considered, which provide estimates of their IR spectra and interpretation of spectral features with respect to molecular structure. Fourth, DT-DFT calculations of UV-Vis spectra are presented. Finally, a conclusion is presented.

Manuscript approved March 7, 2017.

Calculation of Absorption Spectra using DFT

In this section are presented the formal mathematical structure underlying DFT calculations, as well as the procedure for calculation of absorption spectra corresponding to vibrational states. The present study considers DFT calculation of absorption spectra of vibrational states.

The DFT software GAUSSIAN09 (G09) can be used to compute an approximation of the IR absorption spectrum of a molecule or molecules [12]. This program calculates vibrational frequencies by determining second derivatives of the energy with respect to the Cartesian nuclear coordinates, and then transforming to mass-weighted coordinates at a stationary point of the geometry. The IR absorption spectrum is obtained using density functional theory to compute the ground state electronic structure in the Born-Oppenheimer approximation using Kohn-Sham density functional theory [13-18]. GAUSSIAN uses specified orbital basis functions to describe the electronic wavefunctions and density. For a given set of nuclear positions, the calculation directly gives the electronic charge density of the molecule, the potential energy *V,* and the displacements in Cartesian coordinates of each atom. The procedure for vibrational analysis followed in GAUSSIAN is that described in Ref [12]. Reference [18] presents a relatively detailed review of this procedure. A brief description of this procedure is as follows.

The procedure followed by GAUSSIAN is based on the fact the vibrational spectrum depends on the Hessian matrix $\mathbf{f}_{\mathrm{CART}}$, which is constructed using the second partial derivatives of the potential energy *V* with respect to displacements of the atoms in Cartesian coordinates. Accordingly, the elements of the *3N* x *3N* matrix $\mathbf{f}_{\mathrm{CART}}$ are given by

$$f_{\mathrm{CART}ij} = \left(\frac{\partial^2 V}{\partial \xi_i \partial \xi_j} \right)_0 \qquad \text{(Eq 1)}$$

where $\{\xi_1,\xi_2,\xi_3,\xi_4,\xi_5,\xi_6,...,\xi_{3N}\} = \{\Delta x_1,\Delta y_1,\Delta z_1,\Delta x_2,\Delta y_2,\Delta z_2,...,\Delta z_N\}$, which are displacements in Cartesian coordinates, and *N* is the number of atoms. As discussed above, the zero subscript in Eq.(1) indicates that the derivatives are taken at the equilibrium positions of

the atoms, and that the first derivatives are zero. Given the Hessian matrix defined by Eq.(1) the operations for calculation of the vibrational spectrum require that the Hessian matrix Eq.(1) be transformed to mass-weighted Cartesian coordinates according to the relation

$$f_{\mathrm{MWC}ij} = \frac{f_{\mathrm{CART}ij}}{\sqrt{m_i m_j}} = \left(\frac{\partial^2 V}{\partial q_i \partial q_j} \right)_0 \qquad \text{(Eq 2)}$$

where $\{q_1, q_2, q_3, q_4, q_5, q_6, ..., q_{3N}\} = \left\{\sqrt{m_1}\Delta x_1, \sqrt{m_1}\Delta y_1, \sqrt{m}_1\Delta z_1, \sqrt{m}_2\Delta x_2, \sqrt{m_2}\Delta y_2, \sqrt{m_2}\Delta z_2, ..., \sqrt{m_N}\Delta z_N\right\}$ are the mass-weighted Cartesian coordinates. GAUSSIAN computes the energy second derivatives Eq.(2), thus computing the forces for displacement perturbations of each atom along each Cartesian direction. The first derivatives of the dipole moment with respect to atomic positions $\partial\vec{\mu}/\partial\xi_i$ are also computed. Each vibrational eigenmode leads to one peak in the absorption spectrum, at a frequency equal to the mode's eigenfrequency ν_{n0}. The absorption intensity corresponding to a particular eigenmode *n* whose eigenfrequency is ν_{n0} is given by

$$I_n = \frac{\pi}{3c}\left| \sum_{i=1}^{3N} \frac{\partial\vec{\mu}}{\partial\xi_i} l_{\mathrm{CART}in} \right|^2, \qquad \text{(Eq 3)}$$

where $\mathbf{l}_{\mathrm{CART}}$ is the matrix whose elements are the displacements of the atoms in Cartesian coordinates. The matrix $\mathbf{l}_{\mathrm{CART}}$ is determined by the following procedure. First,

$$\mathbf{l}_{\mathrm{CART}} = \mathbf{M}\mathbf{l}_{\mathrm{MWC}}, \qquad \text{(Eq 4)}$$

where $\mathbf{l}_{\mathrm{MWC}}$ is the matrix whose elements are the displacements of the atoms in mass-weighted Cartesian coordinates and **M** is a diagonal matrix defined by the elements

$$M_{ii} = \frac{1}{\sqrt{m_i}}. \qquad \text{(Eq 5)}$$

Proceeding, $\mathbf{l}_{\mathrm{MWC}}$ is the matrix needed to diagonalize $\mathbf{f}_{\mathrm{MWC}}$ defined by Eq.(2) such that

$$(\mathbf{l}_{MWC})^T \mathbf{f}_{MWC} (\mathbf{l}_{MWC}) = \Lambda , \qquad \text{(Eq 6)}$$

where Λ is the diagonal matrix with eigenvalues λ_i. The procedure for diagonalizing Eq.(6) consists of the operations

$$\mathbf{f}_{INT} = (\mathbf{D})^T \mathbf{f}_{MWC} (\mathbf{D}) \qquad \text{(Eq 7)}$$

and

$$(\mathbf{L})^T \mathbf{f}_{MWC} (\mathbf{L}) = \Lambda , \qquad \text{(Eq 8)}$$

where **D** is a matrix transformation to coordinates where rotation and translation have been separated out and **L** is the transformation matrix composed of eigenvectors calculated according to Eq.(8). The eigenfrequencies in units of (cm^{-1}) are calculated using the eigenvalues λ_n by the expression

$$\nu_{n0} = \frac{\sqrt{\lambda_n}}{2\pi c} , \qquad \text{(Eq 9)}$$

where *c* is the speed of light. The elements of $\mathbf{l}_{CART}$ are given by

$$l_{CARTki} = \sum_{j=1}^{3N} \frac{D_{kj} L_{ji}}{\sqrt{m_j}} , \qquad \text{(Eq 10)}$$

where *k, i=1,..., 3N,* and the column vectors of these elements are the normal modes in Cartesian coordinates.

The intensity Eq.(3) must then be multiplied by the number density of molecules to give an absorption-line intensity in the non-interacting molecule approximation. It follows that the absorption spectrum calculated by GAUSSIAN is a sum of delta functions, whose line positions and coefficients correspond to the vibrational-transition frequencies and the absorption-line intensities, respectively. In principle, however, these spectral components must be broadened and shifted to account for anharmonic effects such as finite mode lifetimes and inter-mode couplings.

DFT Calculation of Equilibrium Energies and IR Spectra

Results of a computational investigation using DFT concerning Si_xO_y-nH_2O molecular structures are presented. These results include the relaxed or equilibrium configuration of these molecular structures, ground-state oscillation frequencies and IR intensities for molecular geometries having stable structures, which are calculated by DFT. For these calculations geometry optimization and vibrational analysis was effected using the DFT model B3LYP [19,20] and basis function 6-311+G(d) [21,22]. These basis functions designate the 6-311G basis set supplemented by diffuse function: +, and polarization function: (d), having one set of d functions on heavy atoms [23]. Graphical representations of molecular geometries for a set of Si_xO_y-nH_2O molecular structures at equilibrium are shown in Figs. (1A) through (19A). The equilibrium, or ground-state energies, of these structures are given in Table 1. IR intensities as a function of frequency for these molecular structures are shown in Figs. (1B) through (19B), and given in Tables 2 through 20.

DFT Calculation of UV-Vis Spectra

Results of a computational investigation using TD-DFT concerning Si_xO_y-nH_2O molecular structures are presented. The extension of DFT for the calculation of absorption spectra corresponding to electronic excitation states, which is the formalism of time-dependent density functional theory (TD-DFT) is described in references [24,25]. The results presented include the oscillator strength as a function of excitation energy (within the UV range) for different geometries of the interacting systems associated with stable structures, which are calculated by DFT as described above. The oscillator strengths (UV-Vis intensity) as a function of excitation energy for these molecular structures are given in Table 21.

Conclusion

The DFT and TD-DFT calculated absorption spectra given here provide information concerning molecular level dielectric response structure. The calculations of vibrational and excited state resonance structure associated with Si_xO_y-nH_2O molecular structures using DFT and TD-DFT, respectively, are meant to serve as reasonable estimates of molecular level response characteristics, providing interpretation of dielectric response features with respect to molecular structure, for subsequent adjustment relative to experimental measurements. We have

in this paper studied Si_xO_y-nH_2O molecular structures in order to quantify interpretation of their absorption spectra.

Acknowledgments

Funding for this project was provided by the Office of Naval Research (ONR) through the Naval Research Laboratory's Basic Research Program.

References

[1] W.C. Lu, C.Z. Wang, K.M. Ho, "Medium-Sized Silicon Oxide Clusters by Si_3O_3-ring Assembly," Chem. Phys. Let., 378 (2003) pp. 225-231.

[2] W.C. Lu, C.Z. Wang, V. Nguyen, M.W. Schmidt, M.S. Gordon and K.M. Ho, J. Phys. Chem., A, 107 (2003) 6936-6943.

[3] L.S. Wang, J.B. Nicholas, M. Dupuis, H. Wu, S.D. Colson, Phys. Rev. Lett. 78 (1997) 4450.

[4] L.S. Wang, S.R. Desai, H. Wu, J.B. Nichloas, Z. Phys. D, 40 (1997) 36.

[5] J.R. Chelikowsky, Phys. Rev. B 57 (1998) 3333.

[6] J.A.W. Harkless, D.K. Stilinger, F.H. Stilinger, J. Phys. Chem. 100 (1996) 1098.

[7] S.K. Nayak, B.K. Rao, S.N. Khanna, P. Jena, J. Chem. Phys. 109 (1998) 1245.

[8] T.S. Chu, R.Q. Zhang, J.F. Cheung, J. Phys. Chem. B 105 (2001) 1705.

[9] K. Sen, D. Ghosh, S. Pakhira, T. Banu and A. K. Das, Structure, Stability, and Dissociation of Small Ionic Silicon Oxide Clusters [SiO(n)+(n=3, 4)]: Insight fron Density Functional and Topological Exploration," J. Chem. Phys., 139 (23), 234303 (2013).

[10] R. Kitamura, L. Pilon and M. Jonasz, Optical Constants of Silica Glass From Extreme Ultraviolet to Far Infrared At Near Room Temperature," Applied Optics, Vol. 46, No. 33, (2007) pp. 8118-8133.

[11] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R.

Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.

[12] A. Frisch, M. J. Frisch, F. R. Clemente and G. W. Trucks, *Gaussian 09 User's Reference,* Gaussian Inc., 2009, p, 105-106, online: www.gaussian.com/g_tech/g_ur/g09help.htm

[13] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas," Phys. Rev. **136**, B864, (1964).

[14] W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," Phys. Rev. **140**, A1133 (1965).

[15] R.O. Jones and O. Gunnarson, "The density functional formalism, its applications and prospects," Rev. Mod. Phys. **61**, 689 (1989).

[16] R. M. Martin, *Electronic Structures Basic Theory and Practical Methods*, Cambridge University Press, Cambridge 2004, p. 25.

[17] E. B. Wilson, J. C. Decius and P. C. Cross, *Molecular Vibrations* (McGraw-Hill, New York, 1955).

[18] J.W. Ochterski, "Vibrational Analysis in Gaussian," help@gaussian.com, 1999.

[19] A.D. Becke, "Density-functional Thermochemistry. III. The Role of Exact Exchange", *J. Chem. Phys.* **98**, 5648-5652 (1993).

[20] B. Miehlich, A. Savin, H. Stoll and H. Preuss, "Results Obtained with the Correlation Energy Density Functionals of Becke and Lee, Yang and Parr", Chem. *Phys. Lett.* **157**, 200-206 (1989).

[21] A. D. McLean and G. S. Chandler, "Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18," *J. Chem. Phys.*, **72** 5639-48 (1980).

[22] T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, "Efficient diffuse function-augmented basis-sets for anion calculations. 3. The 3-21+G basis set for 1st-row elements, Li-F," *J. Comp. Chem.*, **4** 294-301, (1983).

[23] M. J. Frisch, J. A. Pople and J. S. Binkley, "Self-Consistent Molecular Orbital Methods. 25. Supplementary Functions for Gaussian Basis Sets," *J. Chem. Phys.*, **80** (1984) 3265-69.

[24] C. A. Ullrich and Z. Yang, "A Brief Compendium of Time-Dependent Density-Functional Theory," Brazilian Journal of Physics 44, 154 (2014)

[25] E. Runge and E.K.U. Gross, "Density-Functional Theory for Time-Dependent Systems," Phys. Rev. Lett., Volume 52, 12, (1984), pp. 997-1000.

Table 1

Label	Cluster	Energy (after OPT)
1-2H_2O	$Si_{14}O_{22}H_4$	-5712.87 a.u.
2-3H_2O	$Si_{12}O_{21}H_6$	-5059.62 a.u.
3-3H_2O	$Si_{12}O_{21}H_6$	-5059.45 a.u.
4-4H_2O	$Si_{12}O_{22}H_8$	-5136.21 a.u.
5-5H_2O	$Si_{12}O_{23}H_{10}$	-5212.70 a.u.
6-6H_2O	$Si_{12}O_{24}H_{12}$	-5289.19 a.u.
7-1H_2O	$Si_{18}O_{25}H_2$	-7095.56 a.u.
8-2H_2O	$Si_{18}O_{26}H_4$	-7172.41 a.u.
9-2H_2Oa	$Si_{18}O_{26}H_4$	-7172.41 a.u.
10-4H_2O	$Si_{18}O_{28}H_8$	-7325.35 a.u.
11-5H_2O	$Si_{18}O_{29}H_{10}$	-7401.82 a.u.
12-7H_2O	$Si_{18}O_{31}H_{14}$	-7554.88 a.u.
13-11H_2O	$Si_{18}O_{35}H_{22}$	-7861.02 a.u.
14-1H_2O	$Si_{18}O_{29}H_2$	-7396.98 a.u.
15-6H_2O	$Si_{18}O_{34}H_{12}$	-7779.75 a.u.
16-12H_2O	$Si_{18}O_{40}H_{24}$	-8238.46 a.u.
17-1H_2O	$Si_{18}O_{31}H_2$	-7548.03 a.u.
18-4H_2O	$Si_{24}O_{36}H_8$	-9665.32 a.u.
19-9H_2O	$Si_{24}O_{45}H_{18}$	-10349.22 a.u.

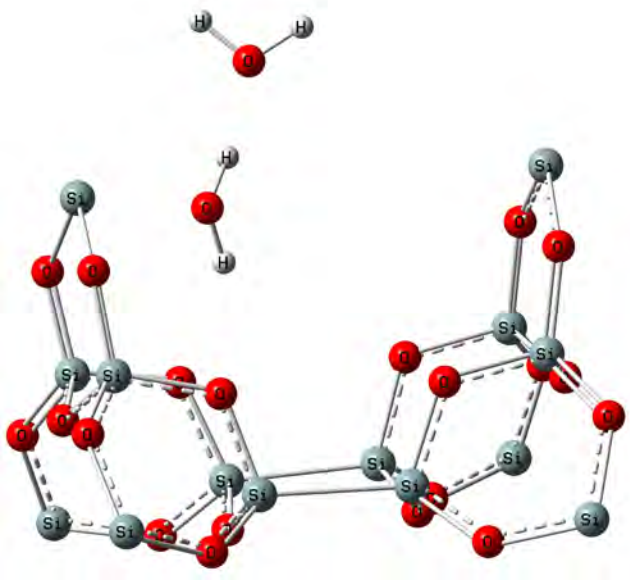

Figure 1A. Equilibrium geometry of molecular cluster 1, $Si_{14}O_{22}H_4$ (Si_xO_y-$2H_2O$).

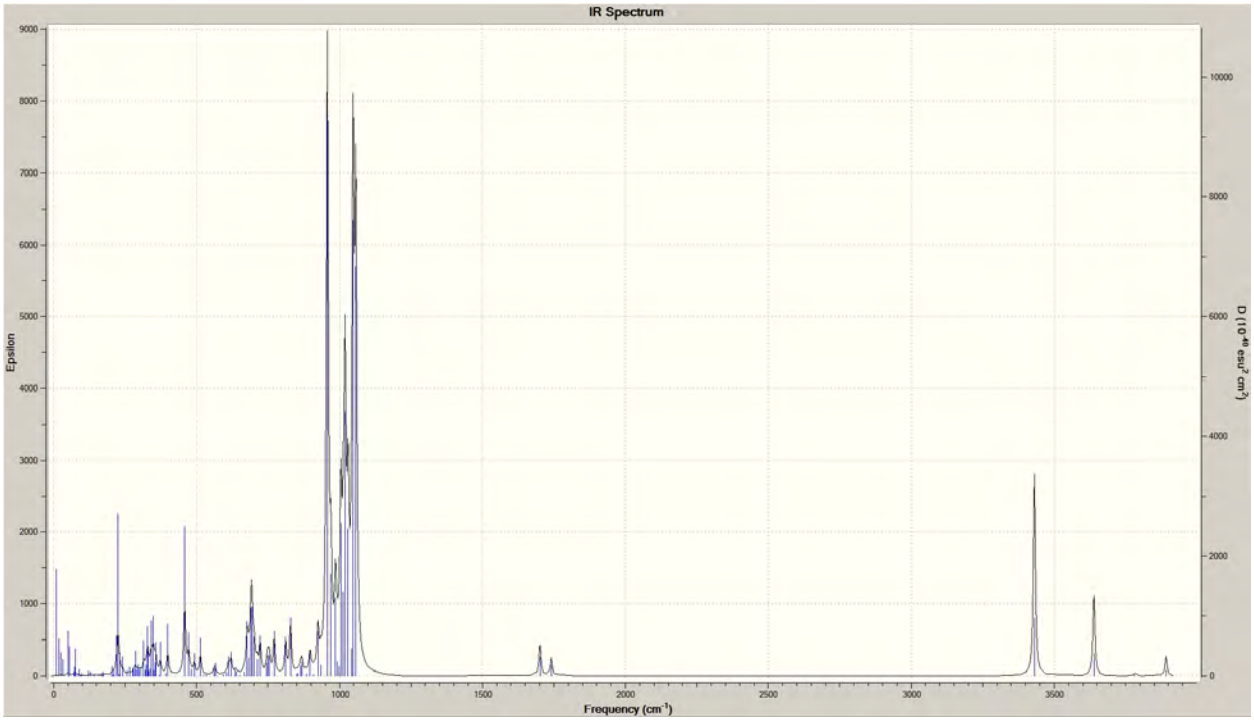

Figure 1B. IR spectrum for molecular cluster 1, $Si_{14}O_{22}H_4$ (Si_xO_y-$2H_2O$).

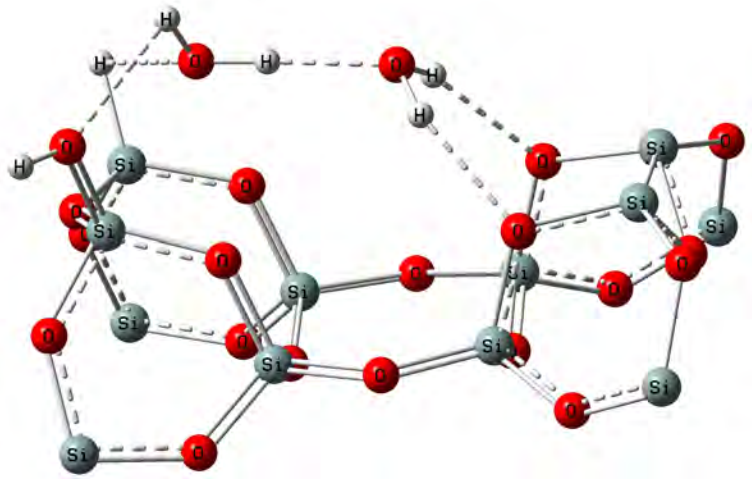

Figure 2A. Equilibrium geometry of molecular cluster 2, $Si_{12}O_{21}H_6$ (Si_xO_y-$3H_2O$).

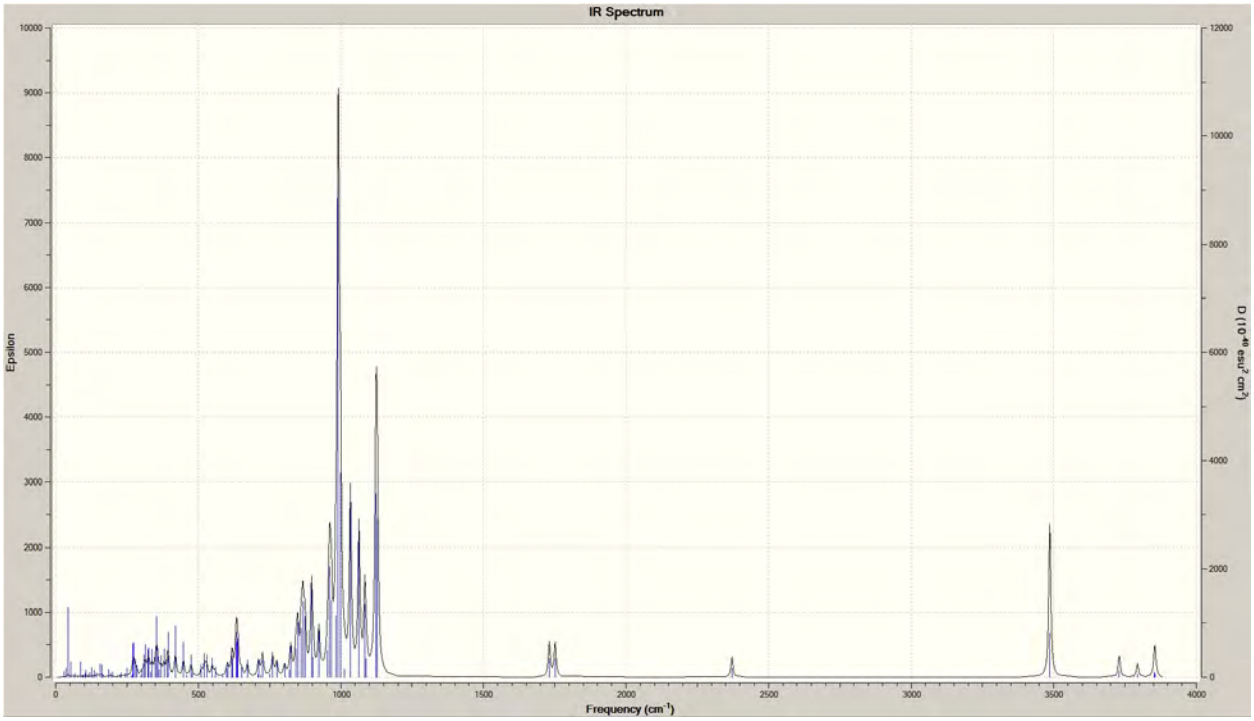

Figure 2B. IR spectrum for molecular cluster 2, $Si_{12}O_{21}H_6$ (Si_xO_y-$3H_2O$).

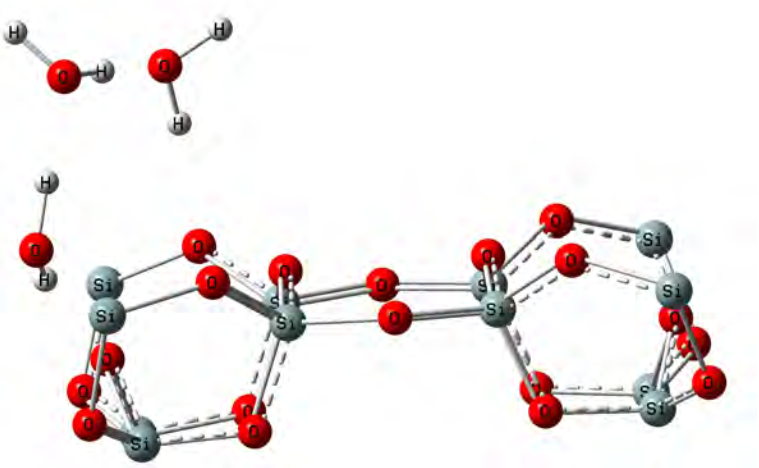

Figure 3A. Equilibrium geometry of molecular cluster 3, $Si_{12}O_{21}H_6$ (Si_xO_y-$3H_2O$).

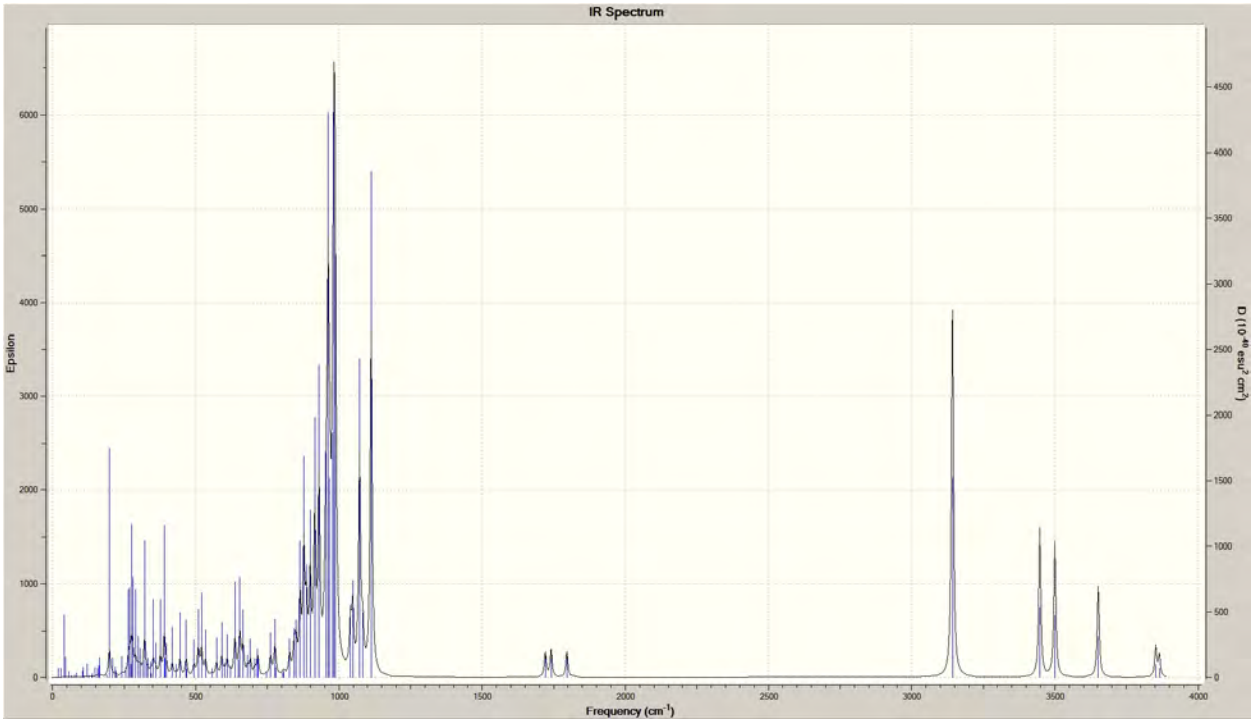

Figure 3B. IR spectrum for $Si_{12}O_{21}H_6$ molecular cluster 3, $Si_{12}O_{21}H_6$ (Si_xO_y-$3H_2O$).

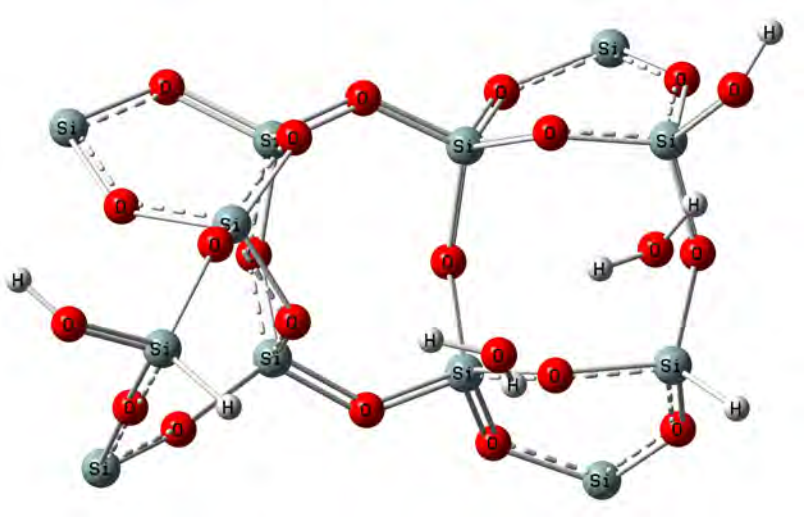

Figure 4A. Equilibrium geometry of molecular cluster 4, $Si_{12}O_{22}H_8$ (Si_xO_y-$4H_2O$).

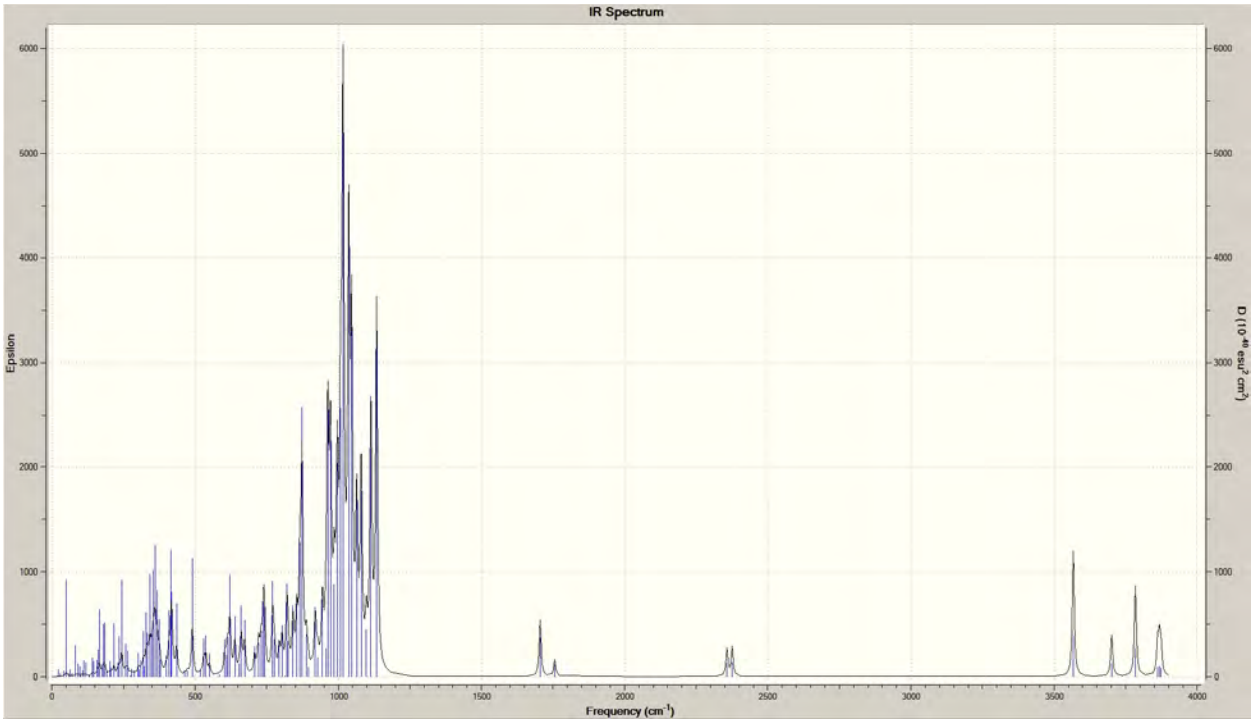

Figure 4B. IR spectrum for molecular cluster 4, $Si_{12}O_{22}H_8$ (Si_xO_y-$4H_2O$).

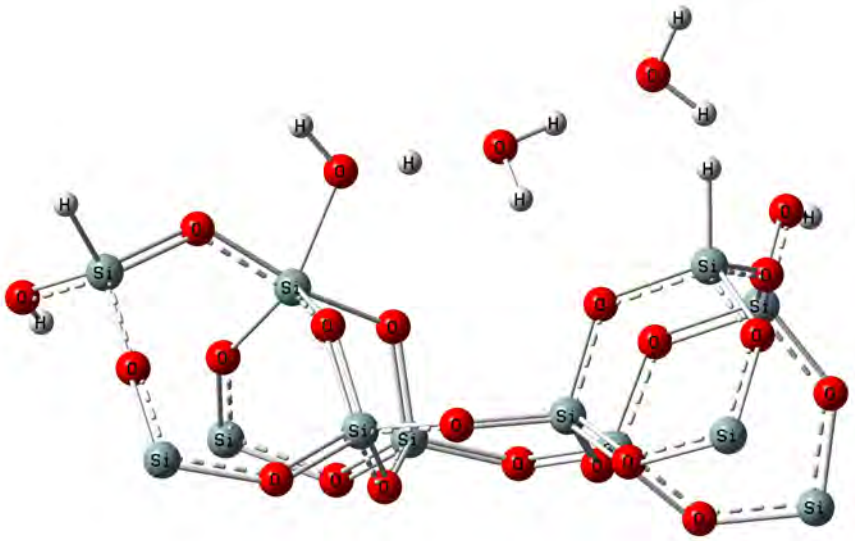

Figure 5A. Equilibrium geometry of molecular cluster 5, $Si_{12}O_{23}H_{10}$ (Si_xO_y-$5H_2O$).

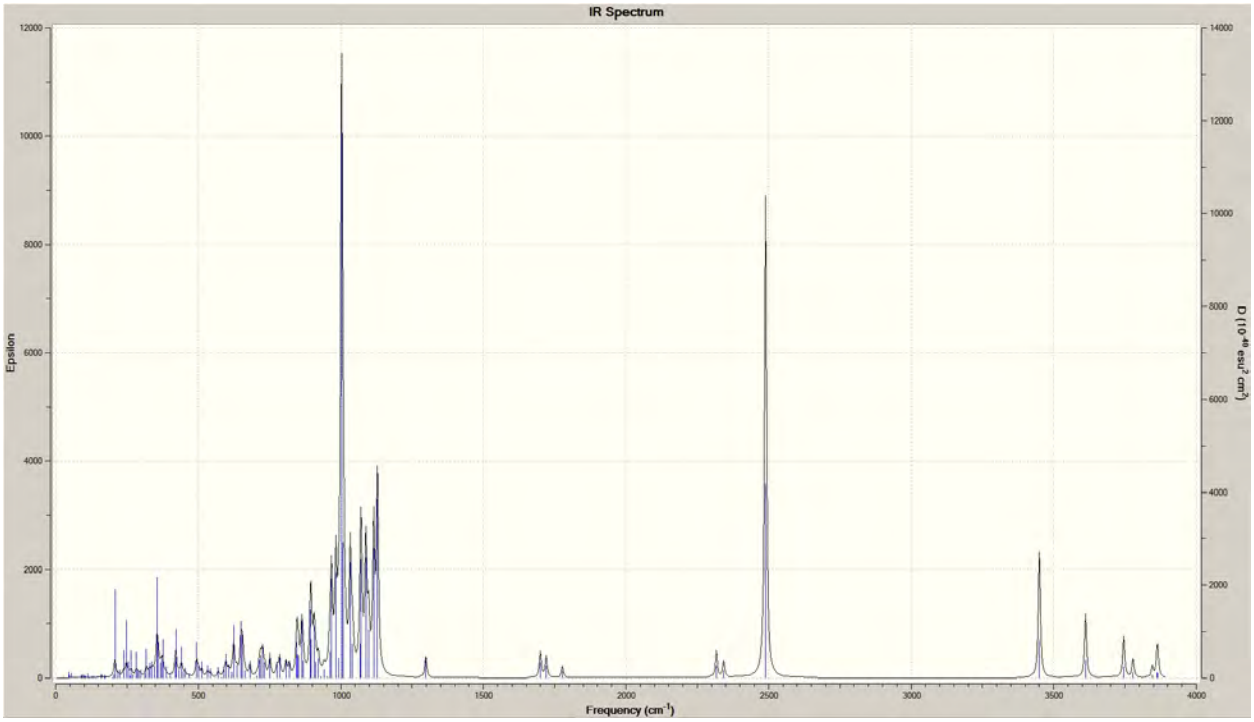

Figure 5B. IR spectrum for molecular cluster 5, $Si_{12}O_{23}H_{10}$ (Si_xO_y-$5H_2O$).

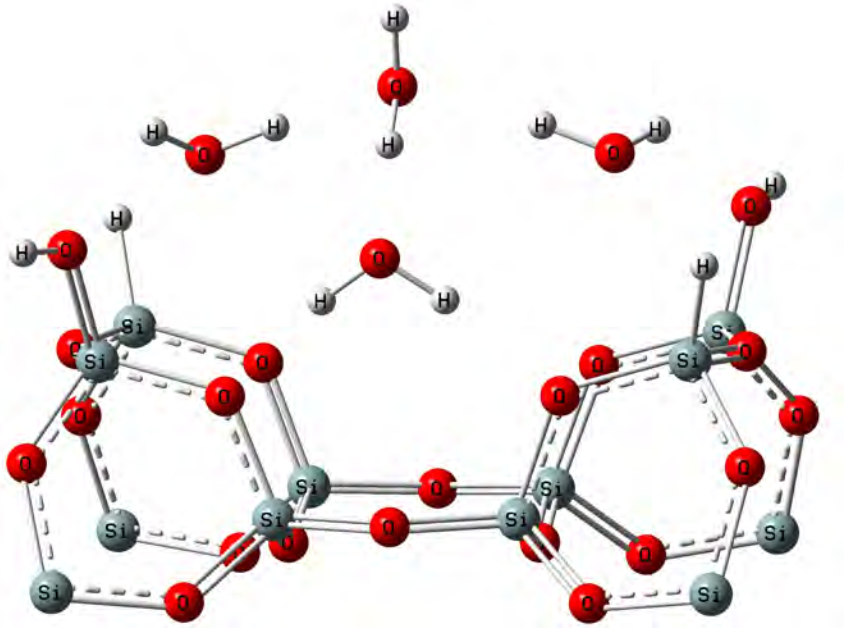

Figure 6A. Equilibrium geometry of molecular cluster 6, $Si_{12}O_{24}H_{12}$ (Si_xO_y-$6H_2O$).

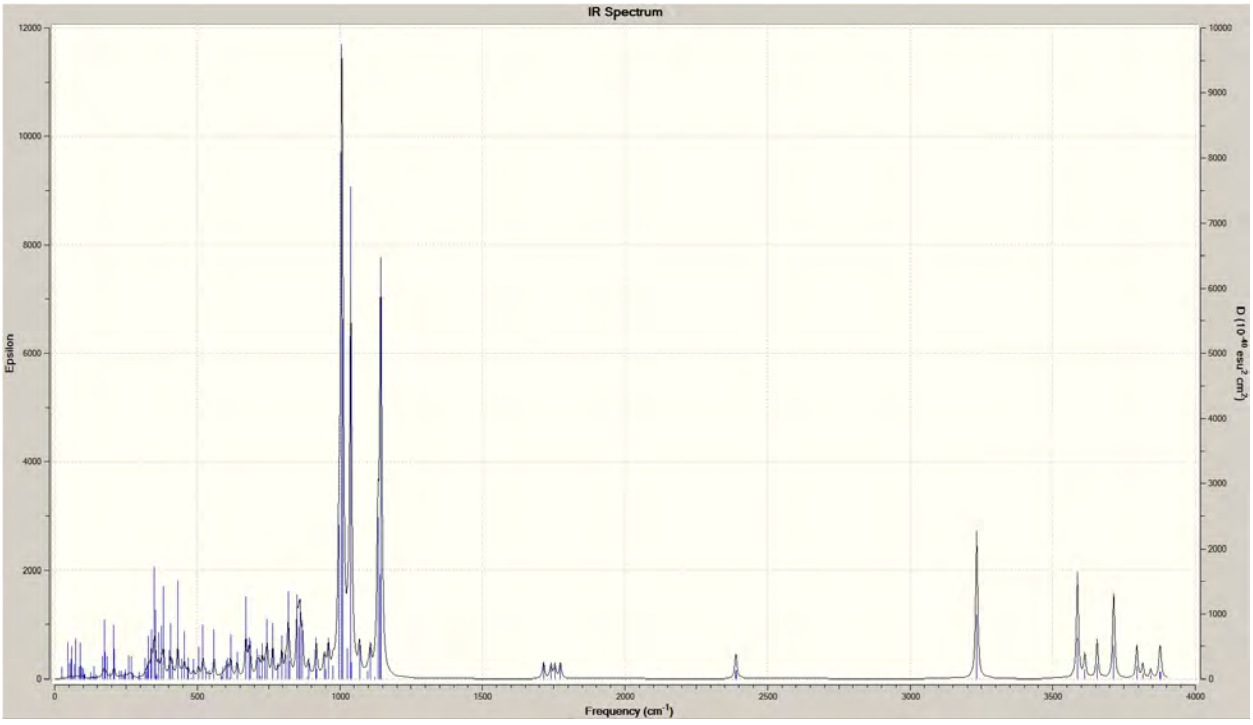

Figure 6B. IR spectrum for molecular cluster 6, $Si_{12}O_{24}H_{12}$ (SixOy-$6H_2O$).

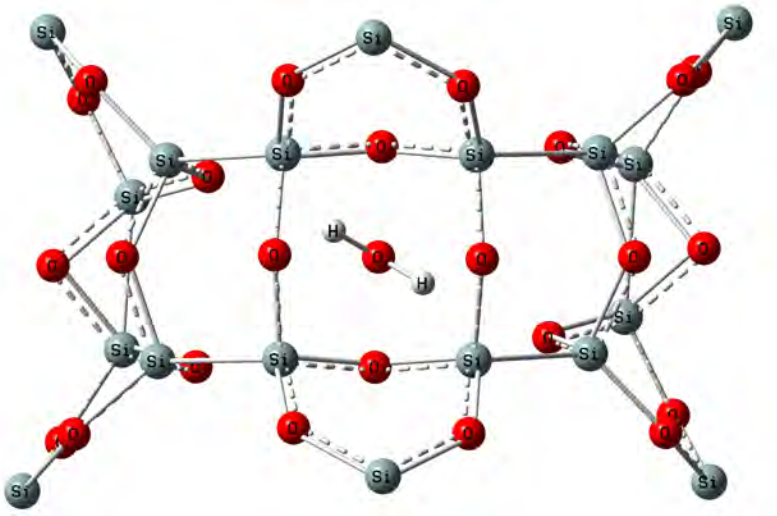

Figure 7A. Equilibrium geometry of molecular cluster 7, $Si_{18}O_{25}H_2$ (Si_xO_y-$1H_2O$).

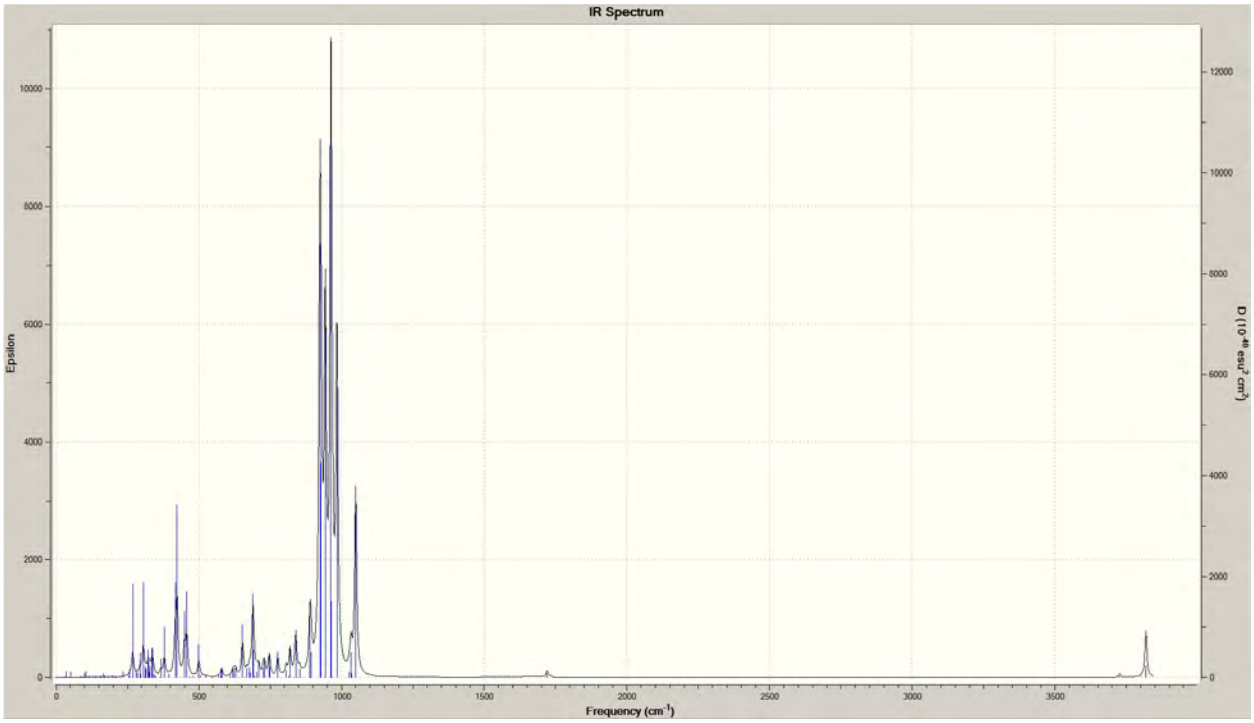

Figure 7B. IR spectrum for molecular cluster 7, $Si_{18}O_{25}H_2$ (Si_xO_y-$1H_2O$).

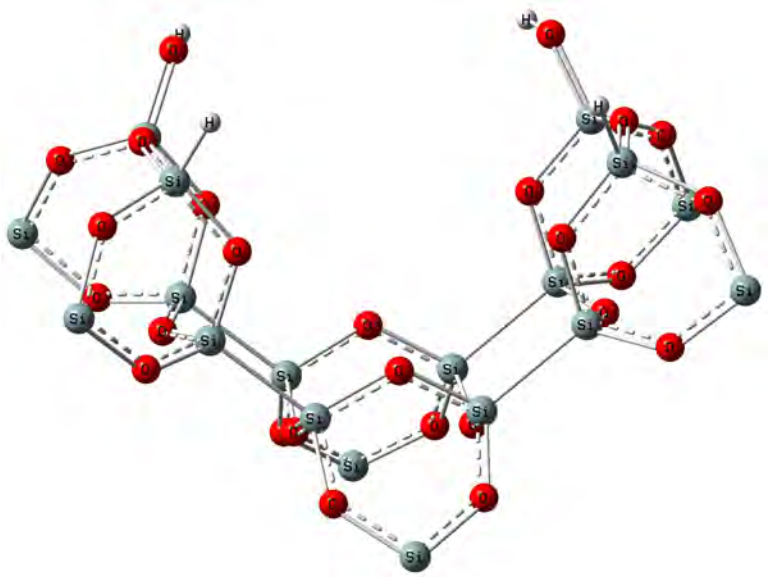

Figure 8A. Equilibrium geometry of molecular cluster 8, $Si_{18}O_{26}H_4$ (Si_xO_y-$2H_2O$).

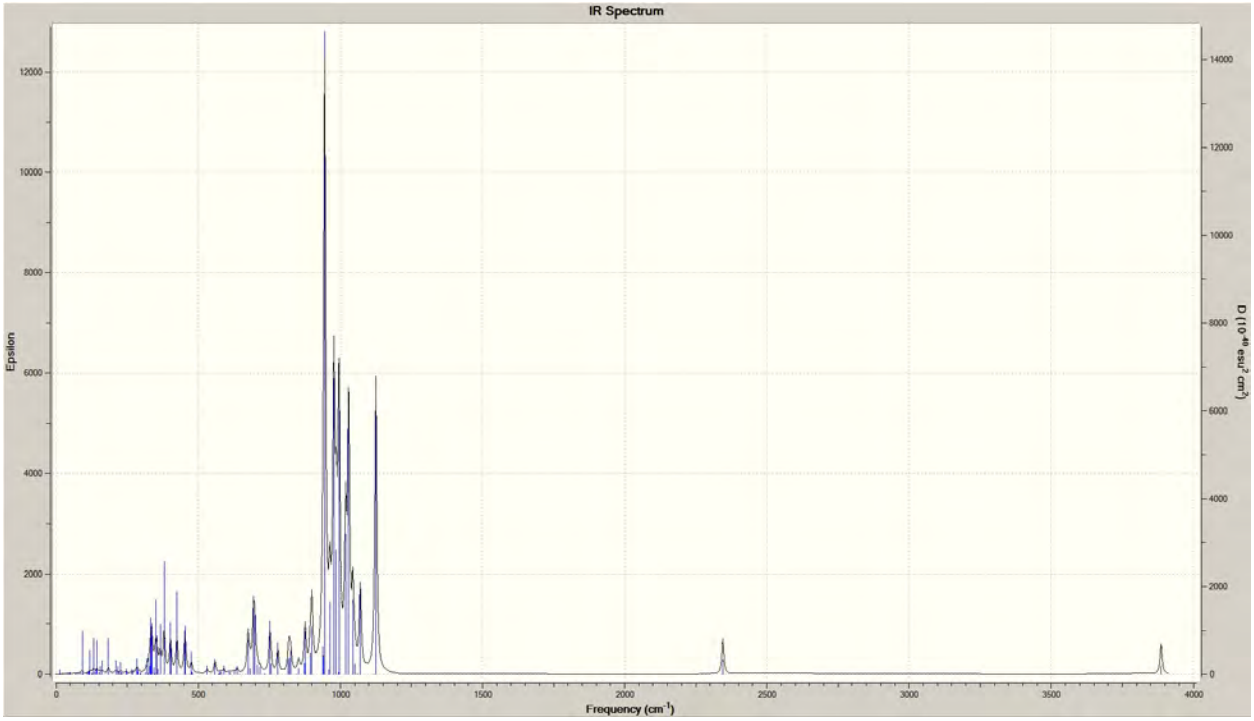

Figure 8B. IR spectrum for molecular cluster 8, $Si_{18}O_{26}H_4$ (Si_xO_y-$2H_2O$).

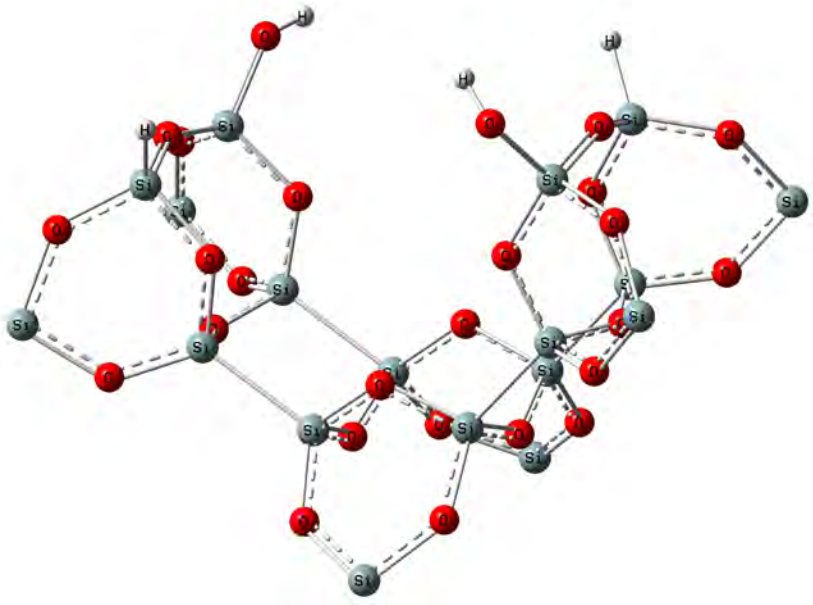

Figure 9A. Equilibrium geometry of molecular cluster 9, $Si_{18}O_{26}H_4$ (Si_xO_y-$2H_2O$).

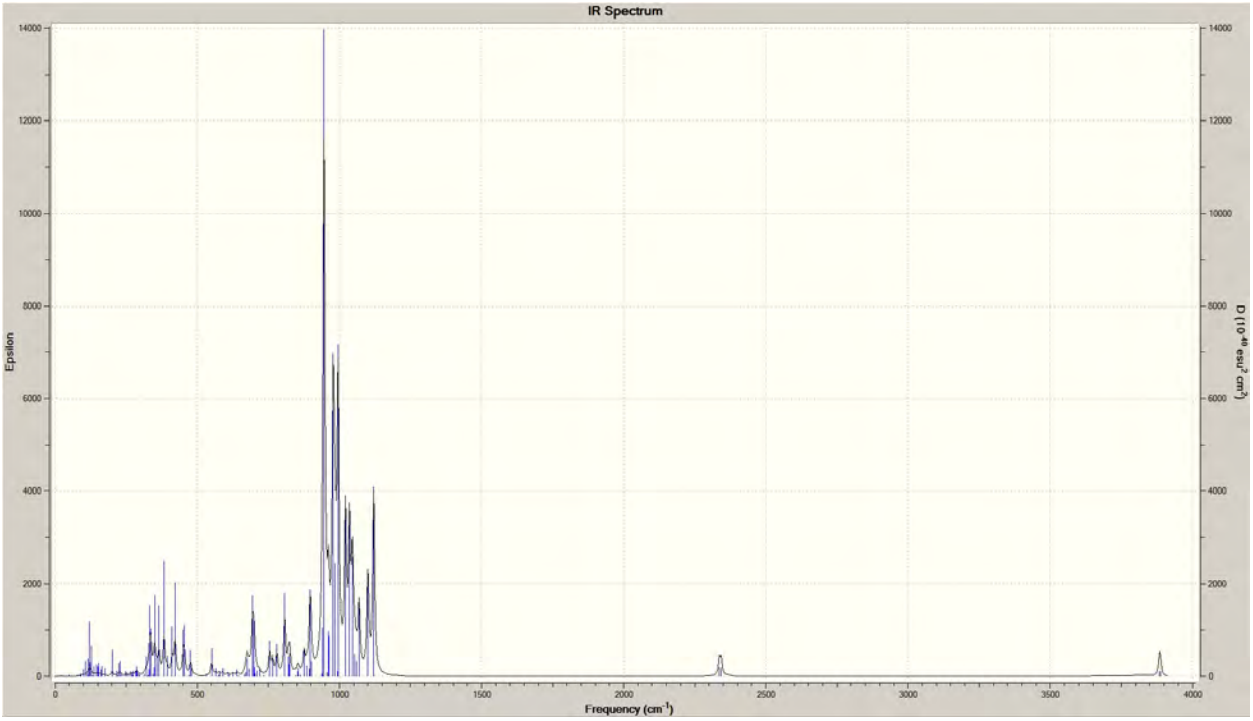

Figure 9B. IR spectrum for molecular cluster 9, $Si_{18}O_{26}H_4$ (Si_xO_y-$2H_2O$).

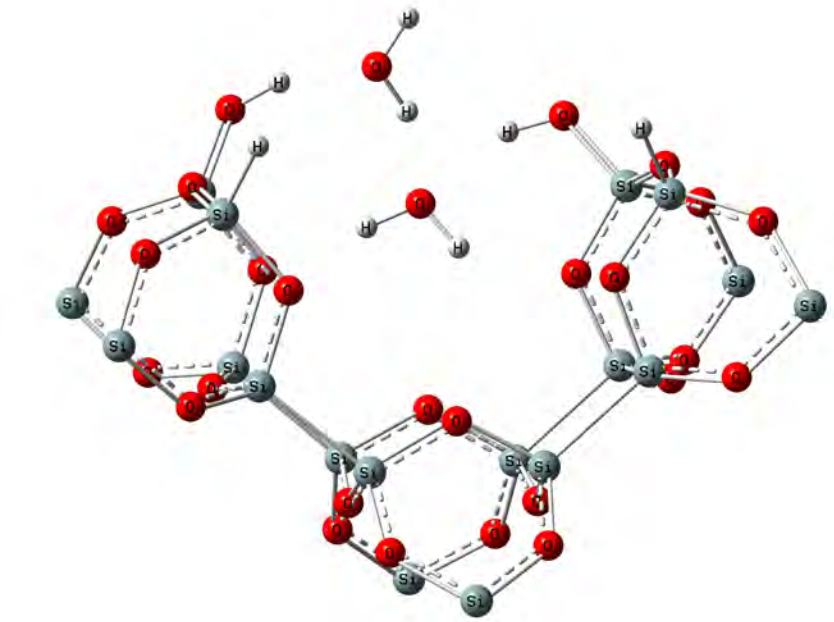

Figure 10A. Equilibrium geometry of molecular cluster 10, $Si_{18}O_{28}H_8$ (Si_xO_y-$4H_2O$).

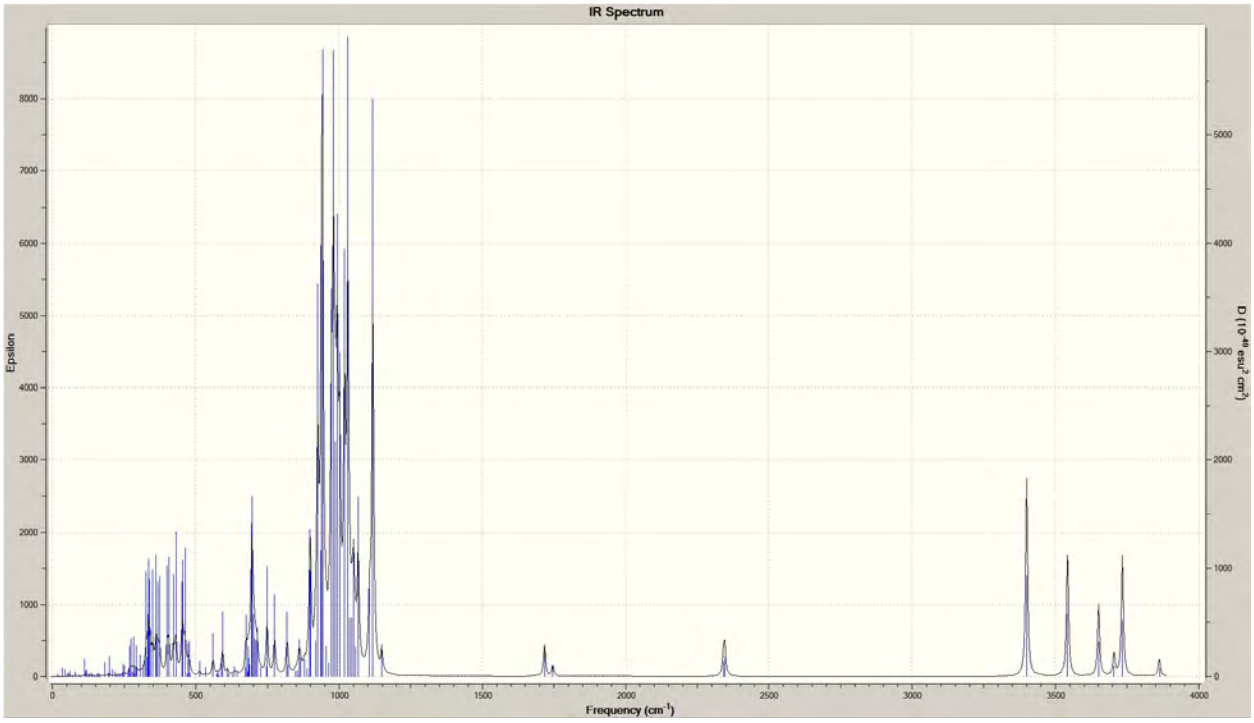

Figure 10B. IR spectrum for molecular cluster 10, $Si_{18}O_{28}H_8$ (Si_xO_y-$4H_2O$).

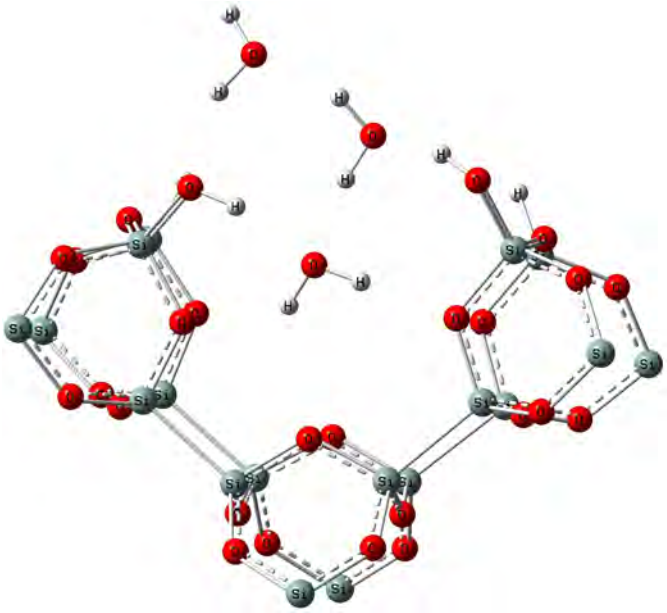

Figure 11A. Equilibrium geometry of molecular cluster 11, $Si_{18}O_{29}H_{10}$ (Si_xO_y-$5H_2O$).

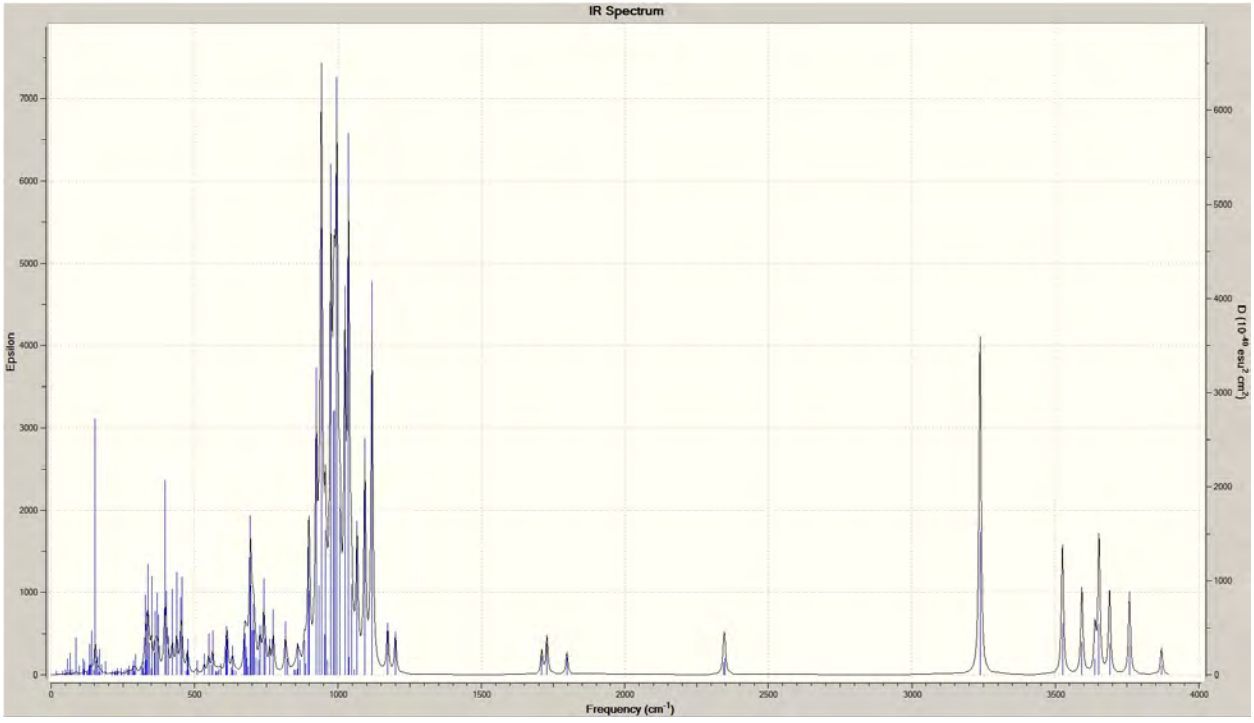

Figure 11B. IR spectrum for molecular cluster 11, $Si_{18}O_{29}H_{10}$ (Si_xO_y-$5H_2O$).

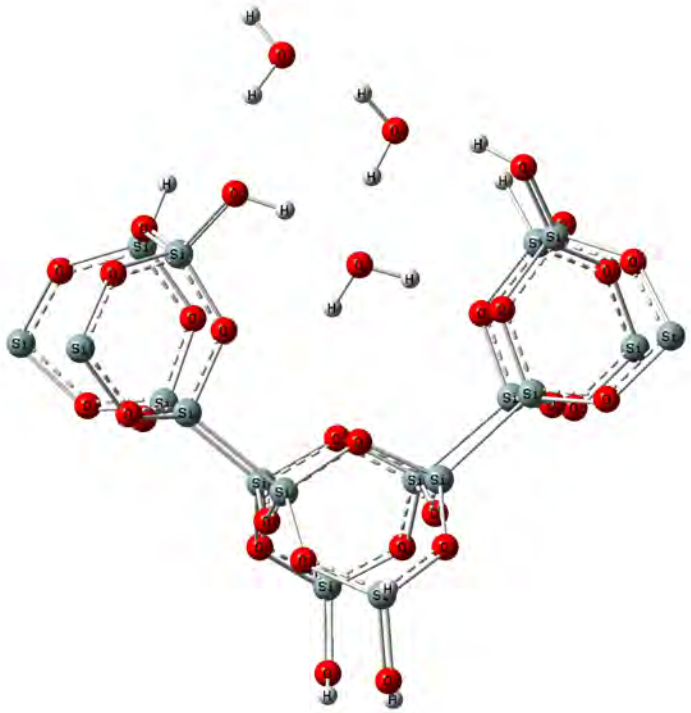

Figure 12A. Equilibrium geometry of molecular cluster 12, $Si_{18}O_{31}H_{14}$ (Si_xO_y-$7H_2O$).

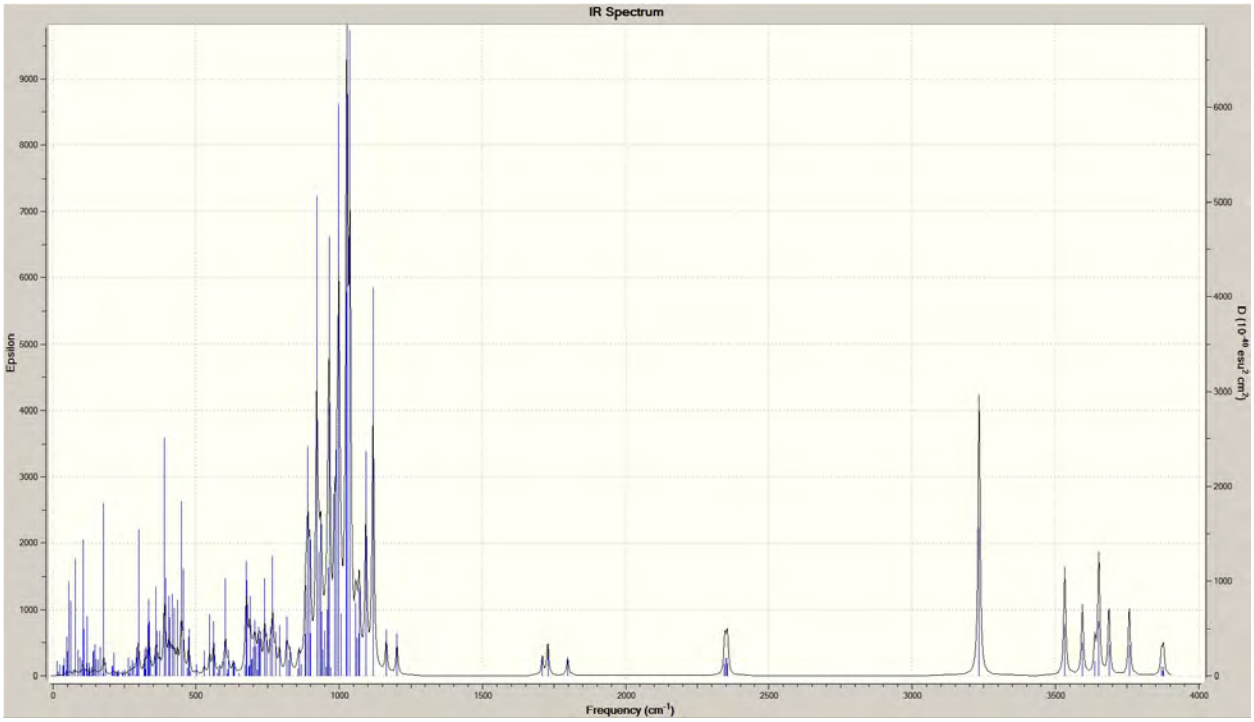

Figure 12B. IR spectrum for molecular cluster 12, $Si_{18}O_{31}H_{14}$ (Si_xO_y-$7H_2O$).

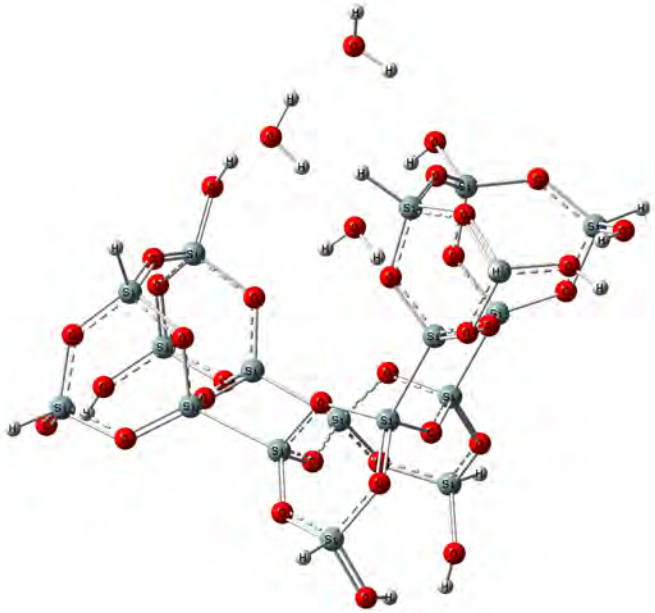

Figure 13A. Equilibrium geometry of molecular cluster 13, $Si_{18}O_{35}H_{22}$ (Si_xO_y-$11H_2O$).

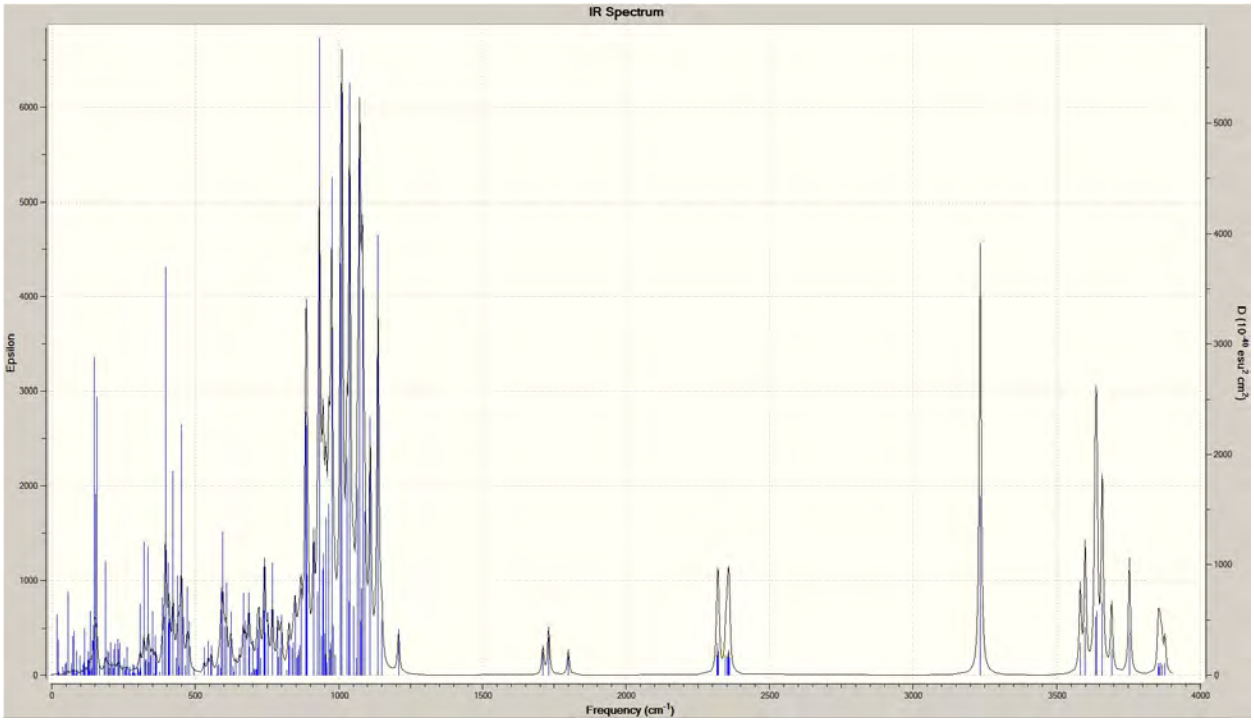

Figure 13B. IR spectrum for molecular cluster 13, $Si_{18}O_{35}H_{22}$ (Si_xO_y-$11H_2O$).

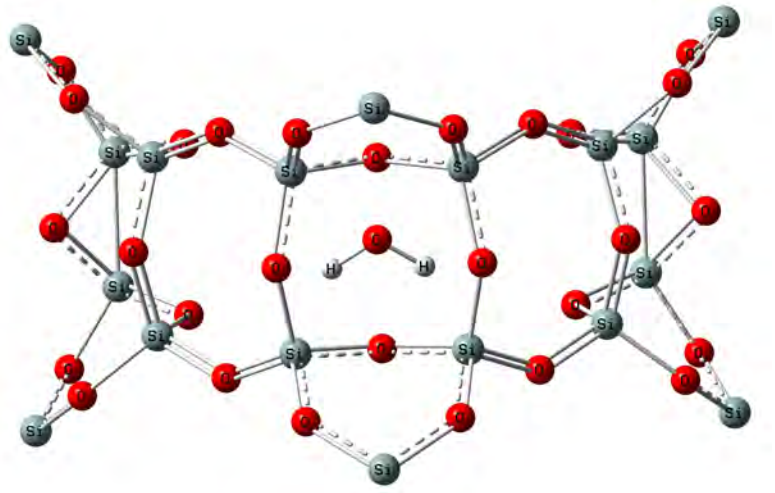

Figure 14A. Equilibrium geometry of molecular cluster 14, $Si_{18}O_{29}H_2$ (Si_xO_y-$1H_2O$).

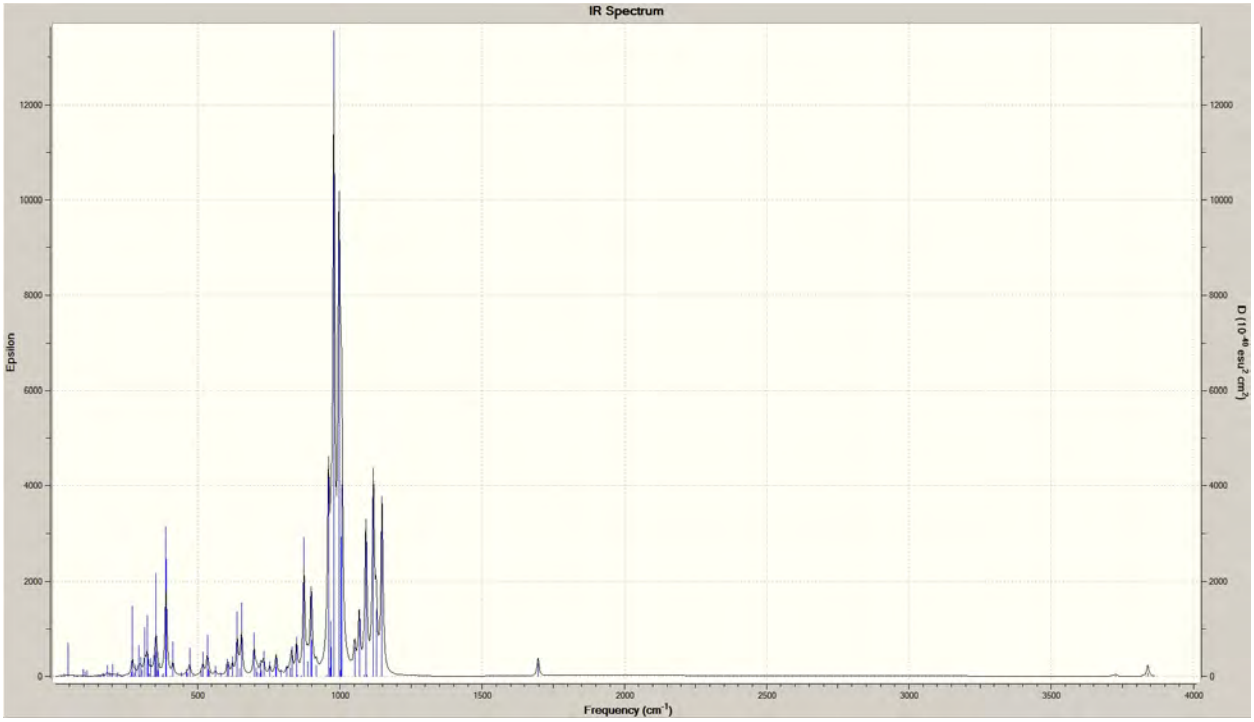

Figure 14B. IR spectrum for molecular cluster 14, $Si_{18}O_{29}H_2$ (Si_xO_y-$1H_2O$).

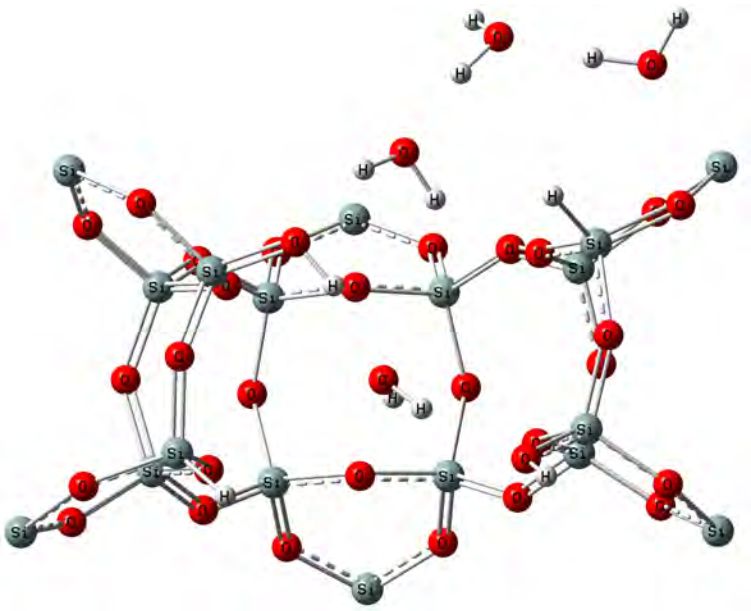

Figure 15A. Equilibrium geometry of molecular cluster 15, $Si_{18}O_{34}H_{12}$ (Si_xO_y-$6H_2O$).

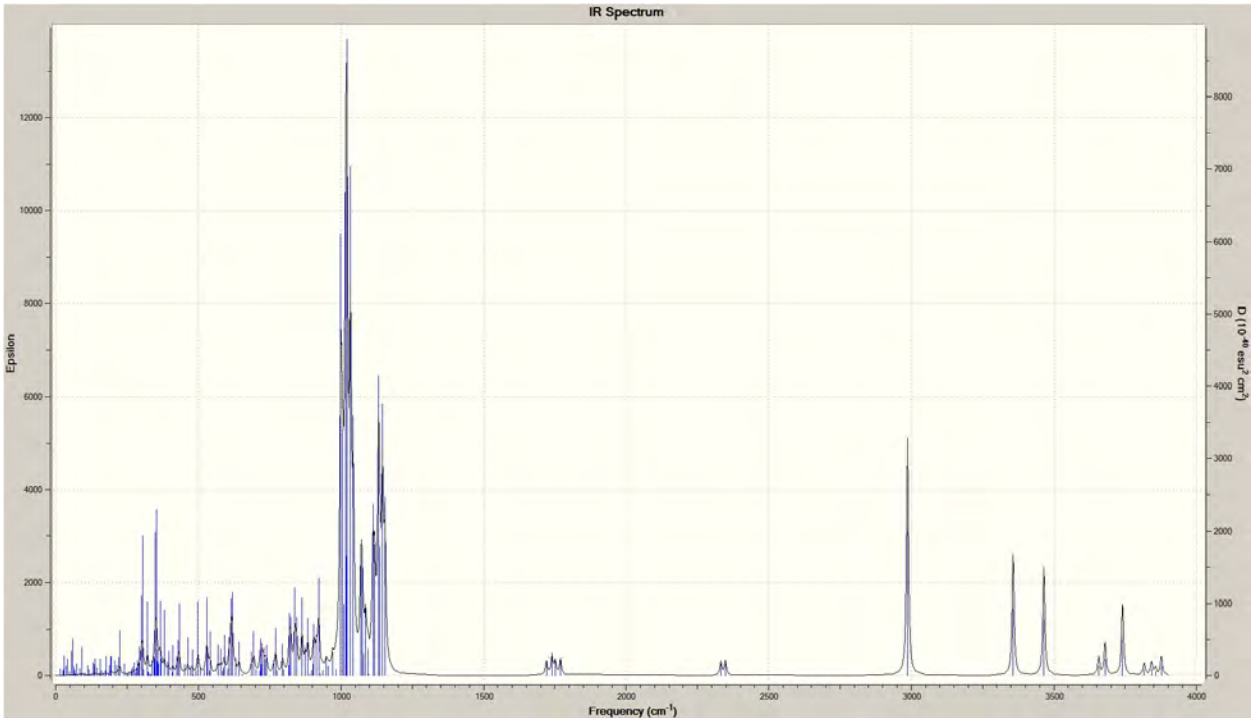

Figure 15B. IR spectrum for molecular cluster 15, $Si_{18}O_{34}H_{12}$ (Si_xO_y-$6H_2O$).

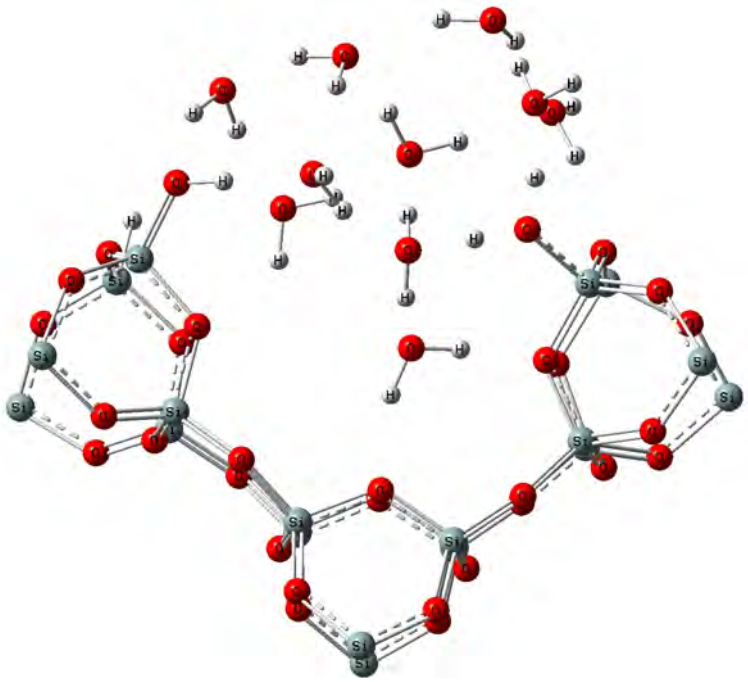

Figure 16A. Equilibrium geometry of molecular cluster 16, $Si_{18}O_{40}H_{24}$ (Si_xO_y-$12H_2O$).

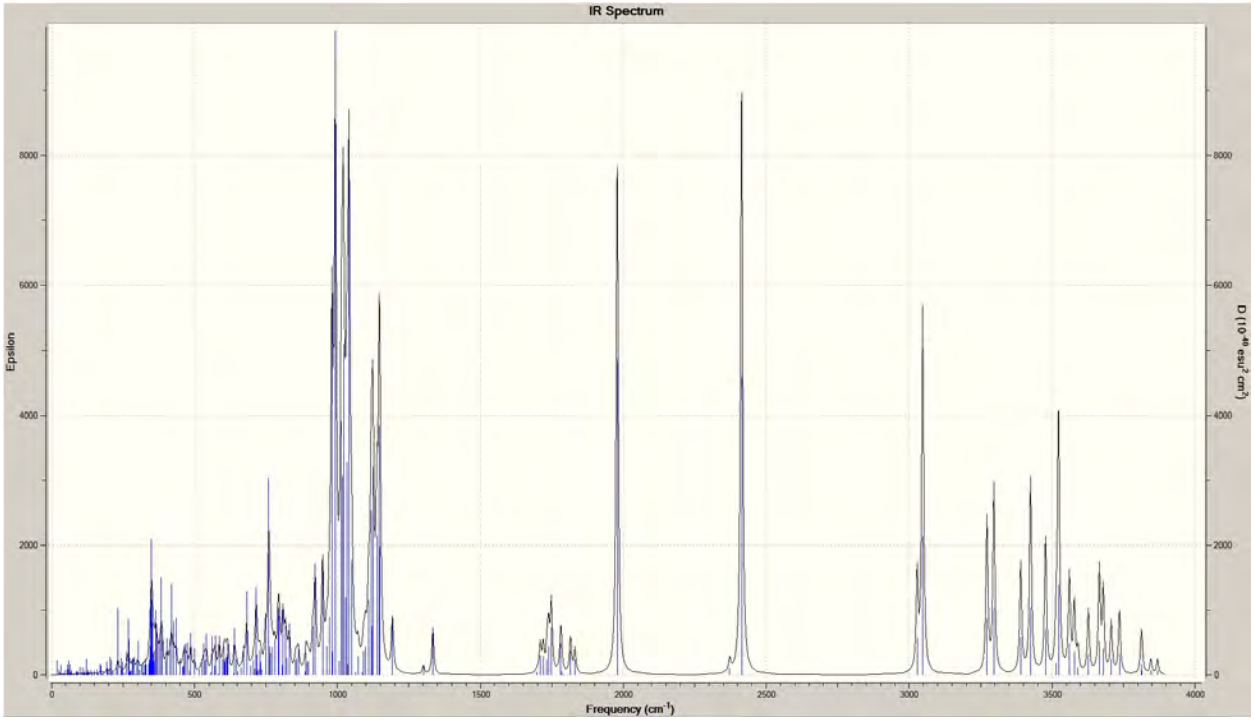

Figure 16B. IR spectrum for molecular cluster 16, $Si_{18}O_{40}H_{24}$ (Si_xO_y-$12H_2O$).

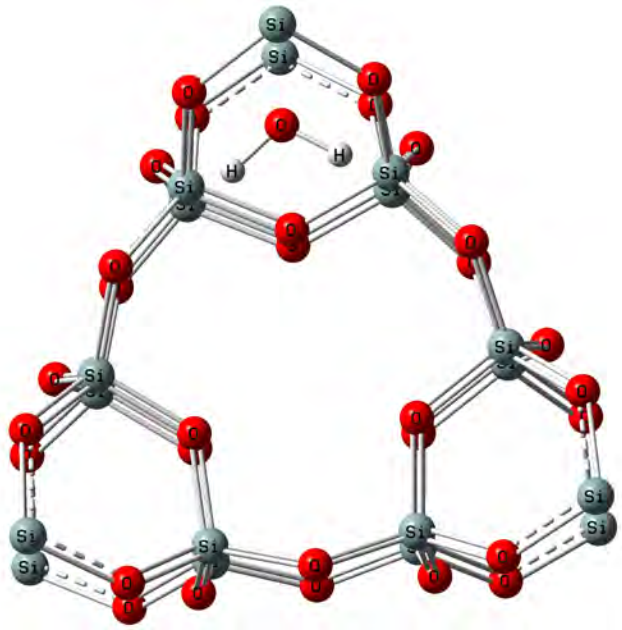

Figure 17A. Equilibrium geometry of molecular cluster 17, $Si_{18}O_{31}H_2$ (Si_xO_y-$1H_2O$).

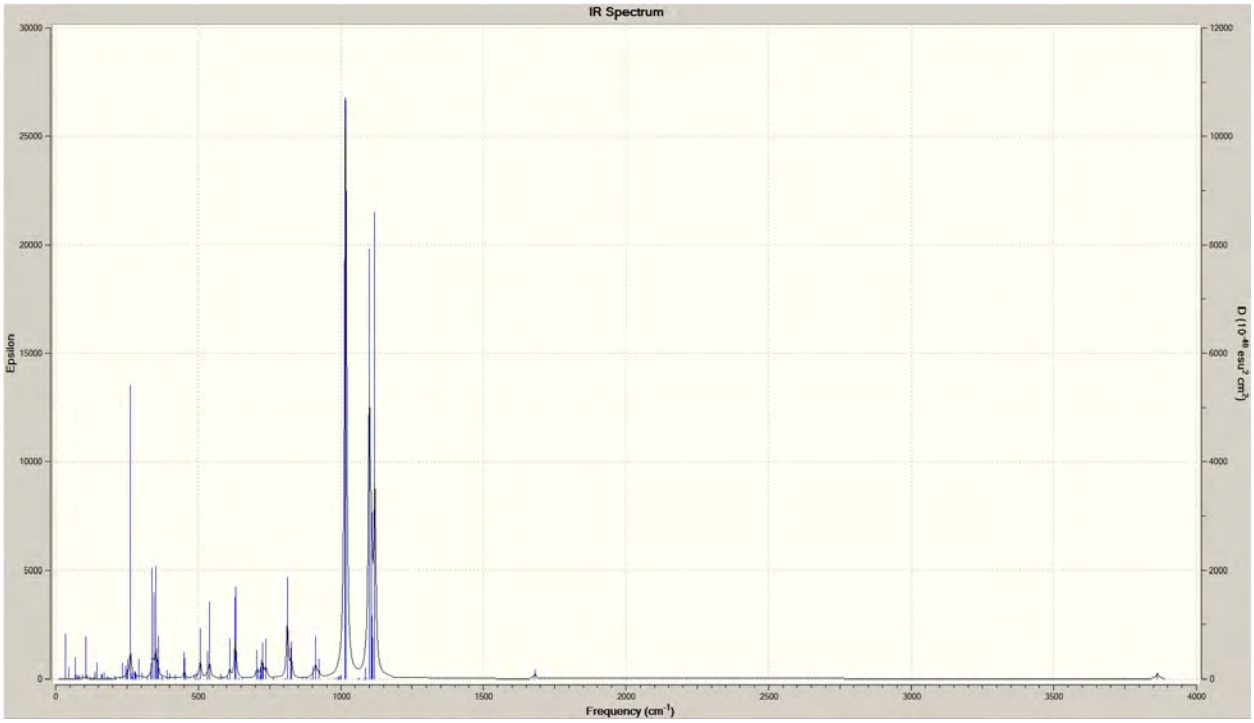

Figure 17B. IR spectrum for molecular cluster 17, $Si_{18}O_{31}H_2$ (Si_xO_y-$1H_2O$).

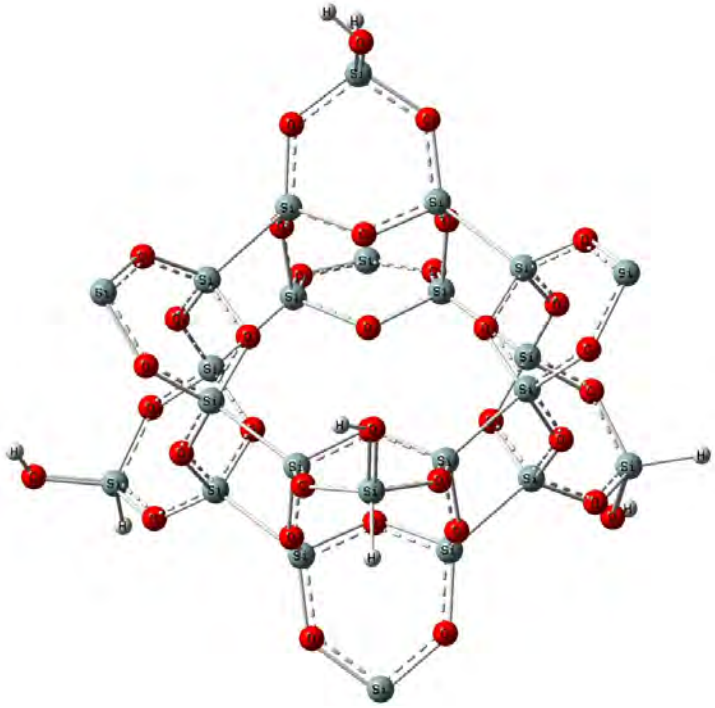

Figure 18A. Equilibrium geometry of molecular cluster18, $Si_{24}O_{36}H_8$ (Si_xO_y-$4H_2O$).

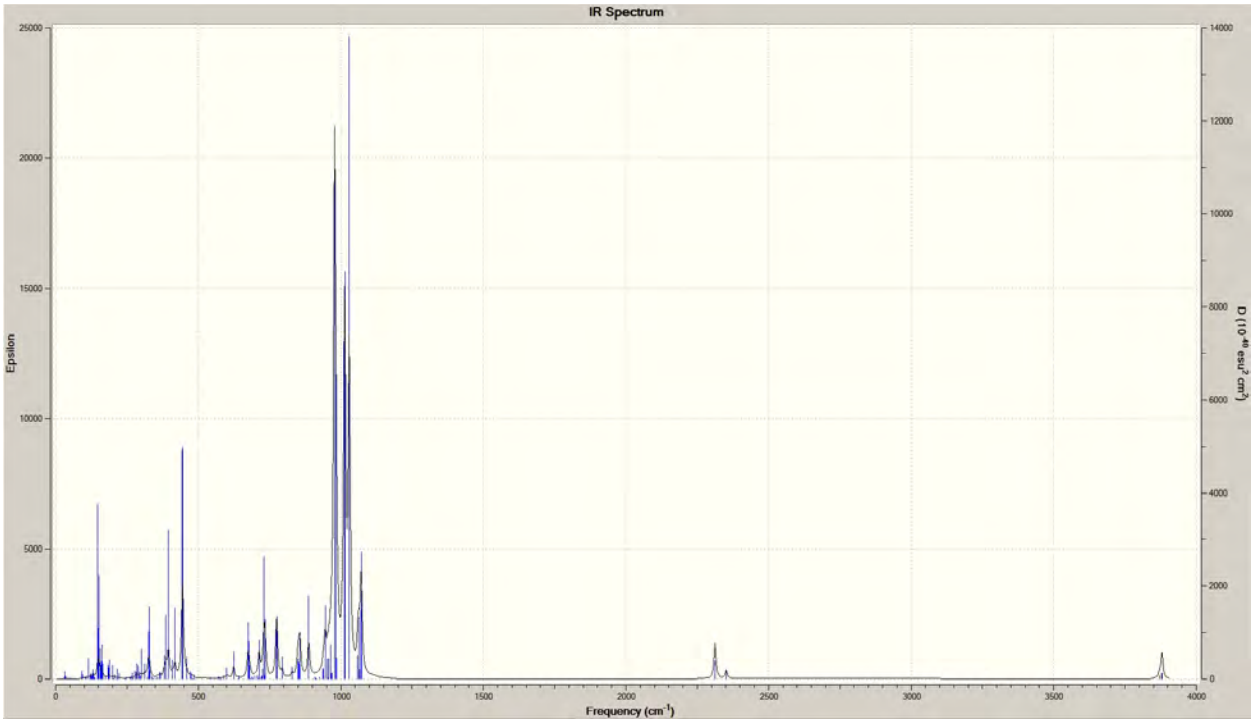

Figure 18B. IR spectrum for molecular cluster18, $Si_{24}O_{36}H_8$ (Si_xO_y-$4H_2O$).

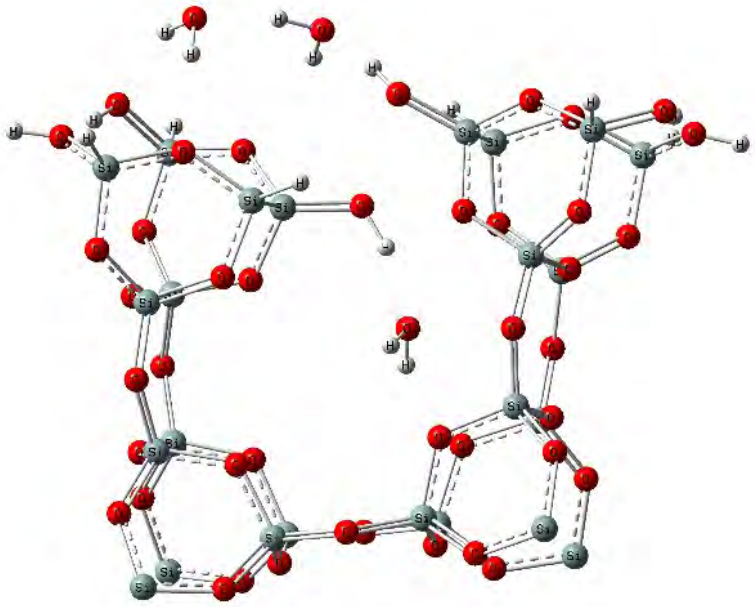

Figure 19A. Equilibrium geometry of molecular cluster 19, $Si_{24}O_{45}H_{18}$ (Si_xO_y-$9H_2O$).

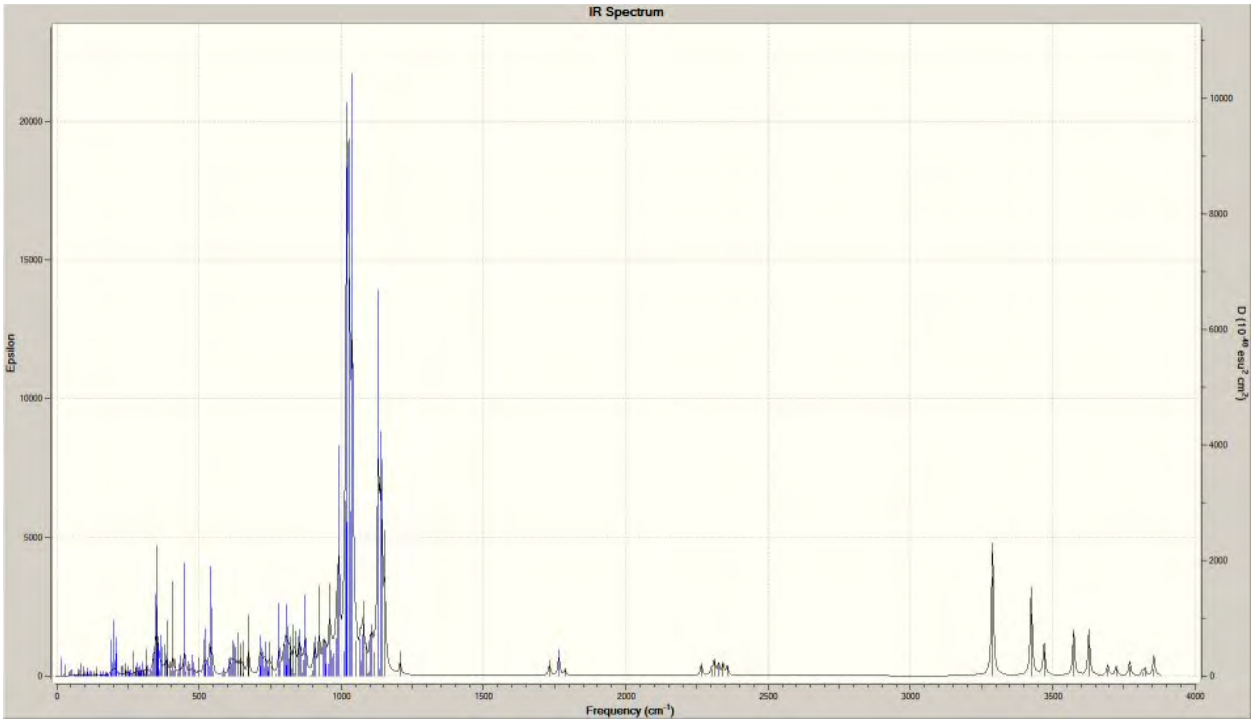

Figure 19B. IR spectrum for molecular cluster 19, $Si_{24}O_{45}H_{18}$ (Si_xO_y-$9H_2O$).

Table 2 (1-2H_2O)
Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	9.365	4.183	39	298.778	7.851	77	690.263	194.499
2	17.479	2.673	40	303.742	9.111	78	693.262	199.852
3	25.683	2.415	41	314.913	46.484	79	700.916	113.200
4	31.955	2.138	42	320.646	7.194	80	711.725	48.511
5	49.304	9.117	43	323.668	13.605	81	722.264	119.748
6	55.075	6.560	44	327.819	66.891	82	745.601	37.426
7	69.891	1.124	45	329.885	33.989	83	749.949	63.038
8	72.637	2.569	46	333.153	6.472	84	754.712	64.384
9	75.822	8.499	47	336.591	9.741	85	771.352	143.178
10	82.908	0.483	48	341.809	78.852	86	811.570	130.056
11	89.882	2.474	49	348.795	86.557	87	828.328	202.030
12	91.586	0.290	50	350.169	7.096	88	848.983	7.351
13	99.394	1.148	51	355.185	19.589	89	854.694	8.067
14	120.798	2.179	52	357.174	50.036	90	862.926	34.490
15	128.931	1.931	53	368.065	1.174	91	868.473	50.648
16	133.997	0.027	54	373.055	53.281	92	883.118	6.611
17	141.269	0.227	55	392.390	3.724	93	896.683	82.614
18	142.766	0.271	56	398.868	86.233	94	909.530	5.453
19	158.589	0.293	57	458.201	285.641	95	924.445	169.706
20	167.549	1.115	58	471.987	85.083	96	934.383	39.170
21	172.863	2.521	59	480.514	13.168	97	957.211	2543.619
22	174.175	0.520	60	491.900	45.952	98	969.647	411.117
23	202.482	0.041	61	513.069	80.408	99	985.648	319.777
24	204.369	7.681	62	523.746	1.665	100	992.693	55.436
25	207.387	0.673	63	534.790	2.877	101	999.623	37.784
26	210.296	5.293	64	560.141	16.568	102	1004.777	642.414
27	220.100	36.721	65	564.808	28.871	103	1013.583	355.291
28	224.929	152.294	66	572.863	0.371	104	1019.315	1126.823
29	229.796	1.404	67	593.720	3.721	105	1029.631	632.778
30	231.419	22.107	68	604.140	7.148	106	1042.736	116.857
31	241.220	19.157	69	612.281	48.539	107	1047.393	1998.642
32	256.431	5.455	70	620.773	60.515	108	1056.825	1809.261
33	265.563	9.141	71	635.500	15.956	109	1701.233	128.543
34	278.159	8.302	72	639.382	10.022	110	1740.912	73.021
35	280.176	9.230	73	651.083	0.960	111	3431.004	828.408
36	285.634	29.756	74	665.908	10.420	112	3639.208	334.830
37	289.424	6.681	75	676.655	152.682	113	3783.087	8.903
38	295.683	13.271	76	682.399	50.906	114	3891.803	78.439

Table 3 (2-3H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	30.035	0.785	38	309.801	31.728	75	724.622	49.374
2	37.341	1.415	39	314.475	47.204	76	726.460	55.211
3	42.689	13.688	40	323.687	41.467	77	750.801	11.045
4	52.039	3.578	41	326.473	44.700	78	761.127	87.802
5	66.660	1.297	42	332.692	8.478	79	775.297	61.931
6	77.122	0.251	43	338.112	44.125	80	802.682	50.065
7	86.860	6.141	44	348.615	33.163	81	820.426	24.360
8	94.595	0.910	45	353.439	100.034	82	824.641	119.151
9	97.297	0.867	46	357.245	47.308	83	842.657	109.589
10	102.584	1.789	47	362.693	12.466	84	848.595	216.622
11	104.849	3.057	48	369.815	36.785	85	860.911	195.665
12	112.399	1.247	49	380.486	49.653	86	866.944	301.378
13	119.449	2.549	50	391.453	43.589	87	874.312	245.499
14	125.509	5.407	51	394.507	81.142	88	897.140	397.644
15	130.424	0.275	52	420.046	99.074	89	903.185	80.923
16	136.304	4.189	53	448.135	73.183	90	923.041	195.333
17	142.427	2.871	54	460.280	3.658	91	953.891	118.700
18	155.978	9.455	55	474.185	49.463	92	960.485	488.001
19	162.820	8.984	56	479.128	8.123	93	966.121	342.731
20	165.662	1.350	57	510.673	29.339	94	982.334	280.467
21	185.845	6.267	58	522.235	56.969	95	990.797	2503.591
22	192.017	3.312	59	529.692	54.315	96	998.746	943.564
23	199.657	4.797	60	548.910	48.752	97	1011.975	38.127
24	216.432	0.457	61	559.322	24.600	98	1033.539	808.130
25	225.856	2.556	62	584.517	6.673	99	1063.611	664.671
26	229.682	4.888	63	600.249	21.630	100	1083.934	365.842
27	242.531	3.833	64	603.174	37.809	101	1088.973	92.048
28	251.402	9.716	65	618.302	59.400	102	1123.055	954.751
29	263.519	1.430	66	618.911	53.434	103	1127.465	827.748
30	267.595	3.371	67	632.753	130.070	104	1731.208	154.274
31	271.485	41.891	68	634.970	103.351	105	1751.527	155.472
32	273.262	43.639	69	639.149	112.133	106	2371.754	91.170
33	279.163	23.192	70	651.700	28.471	107	3486.350	703.287
34	279.850	3.770	71	672.348	52.841	108	3729.931	97.129
35	285.007	15.774	72	709.129	8.958	109	3793.815	59.775
36	298.680	3.093	73	711.557	61.334	110	3853.701	98.185
37	301.978	9.887	74	719.765	5.528	111	3856.199	61.780

Table 4 (3-3H_2O)
Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	20.815	0.365	38	305.694	10.549	75	715.466	38.533
2	28.184	0.479	39	314.219	10.366	76	717.877	29.123
3	39.838	4.797	40	321.095	84.076	77	747.707	7.441
4	45.893	1.830	41	322.146	32.531	78	761.445	65.574
5	55.375	0.618	42	328.909	8.761	79	776.060	86.847
6	65.208	0.244	43	334.019	12.745	80	779.632	15.052
7	76.347	0.351	44	342.085	10.194	81	803.039	7.368
8	83.484	0.772	45	344.570	2.526	82	807.454	10.312
9	104.073	1.310	46	352.101	52.446	83	827.737	61.170
10	107.184	2.084	47	360.106	23.872	84	843.259	79.607
11	112.006	0.332	48	376.137	55.938	85	849.773	93.298
12	119.857	3.132	49	389.920	113.119	86	864.051	224.984
13	127.027	0.506	50	391.356	14.532	87	877.269	371.674
14	135.704	0.457	51	396.715	25.830	88	886.541	190.707
15	138.512	1.055	52	417.936	40.273	89	899.511	287.535
16	148.077	2.827	53	431.720	10.774	90	915.327	454.978
17	156.219	2.767	54	444.491	55.057	91	930.213	555.557
18	161.548	3.681	55	466.296	51.171	92	954.125	411.577
19	164.335	6.332	56	468.723	7.472	93	961.892	1038.382
20	188.985	0.928	57	493.788	35.589	94	967.352	368.915
21	198.481	86.987	58	508.567	18.484	95	978.700	457.985
22	208.615	8.156	59	508.707	66.402	96	982.648	1148.671
23	210.282	2.162	60	519.701	84.040	97	986.723	914.214
24	218.793	4.474	61	533.663	48.544	98	1040.118	143.884
25	220.276	2.878	62	556.033	9.986	99	1047.954	194.674
26	226.487	0.808	63	572.455	44.062	100	1071.745	651.659
27	242.554	10.099	64	590.426	62.020	101	1082.792	134.371
28	255.004	4.643	65	600.587	16.361	102	1112.503	1075.033
29	264.582	44.324	66	609.403	50.765	103	1720.557	76.667
30	269.513	46.213	67	620.502	13.981	104	1740.728	90.113
31	274.153	6.774	68	636.505	116.224	105	1796.007	79.792
32	275.327	80.579	69	649.292	22.199	106	3142.615	1197.570
33	276.768	0.195	70	654.312	125.612	107	3447.681	460.359
34	279.997	53.726	71	664.917	86.659	108	3500.264	417.013
35	289.619	48.769	72	681.013	29.969	109	3651.895	289.219
36	298.340	23.419	73	690.539	50.844	110	3852.658	95.740
37	304.518	16.912	74	705.955	25.341	111	3865.099	69.779

Table 5 (4-4H_2O)
Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	22.552	0.366	41	319.588	34.914	81	770.816	175.950
2	28.457	0.201	42	322.908	7.708	82	777.104	68.763
3	40.284	0.569	43	329.449	50.757	83	793.640	68.723
4	50.377	11.686	44	334.133	34.903	84	804.030	98.366
5	58.594	0.446	45	342.098	84.247	85	813.905	1.375
6	64.532	1.104	46	349.177	39.784	86	820.580	183.164
7	70.563	0.483	47	354.184	90.195	87	825.225	69.372
8	82.553	6.152	48	360.464	112.763	88	842.046	143.910
9	91.746	2.876	49	361.752	32.866	89	854.973	150.362
10	98.783	2.400	50	367.917	76.104	90	866.292	278.133
11	101.033	0.303	51	375.027	51.804	91	873.519	561.709
12	106.210	1.571	52	379.960	15.166	92	888.573	90.697
13	112.156	4.324	53	398.905	20.252	93	894.782	20.194
14	117.250	3.955	54	408.625	64.512	94	919.822	152.726
15	129.609	0.186	55	416.604	127.004	95	928.817	42.534
16	131.151	0.561	56	418.880	84.831	96	944.785	184.786
17	140.568	6.469	57	435.519	76.532	97	957.258	63.808
18	145.999	5.498	58	464.321	5.240	98	963.443	678.209
19	158.256	6.410	59	472.313	6.660	99	972.739	622.418
20	162.906	10.315	60	472.907	3.801	100	985.581	217.308
21	166.155	26.885	61	490.285	139.106	101	996.411	508.460
22	175.604	4.992	62	518.983	9.036	102	1008.372	646.614
23	180.120	22.527	63	530.240	47.857	103	1016.715	1538.249
24	184.895	23.750	64	537.547	52.644	104	1036.543	1203.907
25	192.200	2.501	65	549.779	29.524	105	1046.614	876.410
26	201.938	7.357	66	584.577	2.394	106	1064.313	448.909
27	206.000	4.509	67	603.575	53.738	107	1080.045	573.383
28	216.478	27.278	68	610.545	32.707	108	1098.166	124.490
29	229.595	7.665	69	613.894	57.273	109	1114.228	748.958
30	234.599	22.752	70	621.589	151.690	110	1134.058	1015.499
31	243.918	56.512	71	638.819	92.371	111	1705.341	157.555
32	244.928	7.174	72	654.442	20.547	112	1756.266	47.423
33	258.404	20.241	73	661.177	113.180	113	2357.554	75.968
34	264.793	16.004	74	673.195	91.047	114	2375.758	81.979
35	274.128	0.738	75	707.855	50.592	115	3567.192	349.761
36	278.536	4.888	76	721.317	58.194	116	3701.310	115.561
37	288.214	4.336	77	722.152	28.601	117	3784.056	251.412
38	302.009	16.844	78	730.214	79.626	118	3861.664	88.748
39	304.633	4.926	79	738.205	132.886	119	3867.955	95.699
40	310.237	12.149	80	742.171	155.427	120	3873.773	76.538

Table 6 (5-5H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	28.509	0.149	44	329.730	26.299	87	807.395	82.888
2	34.470	0.030	45	337.431	30.178	88	819.164	68.515
3	40.014	0.040	46	338.560	11.877	89	845.448	162.283
4	45.566	1.420	47	345.865	21.574	90	847.316	108.068
5	48.699	0.683	48	354.946	193.516	91	851.263	102.923
6	55.306	0.144	49	359.172	81.499	92	863.161	262.051
7	55.901	1.340	50	366.775	30.157	93	867.726	80.457
8	68.172	0.147	51	371.008	44.046	94	893.761	327.657
9	89.183	1.546	52	375.537	78.702	95	895.990	187.783
10	92.934	1.062	53	387.088	22.980	96	906.146	252.631
11	96.222	1.755	54	402.755	9.969	97	911.638	77.509
12	99.917	1.193	55	419.622	36.192	98	921.189	97.331
13	103.245	1.173	56	421.410	111.225	99	929.893	5.905
14	112.596	2.464	57	431.293	18.300	100	941.033	44.071
15	119.858	0.373	58	440.768	73.803	101	952.084	7.267
16	126.422	0.929	59	446.904	15.189	102	961.431	132.439
17	132.577	1.595	60	454.944	23.987	103	967.136	517.352
18	140.119	0.156	61	468.541	10.229	104	982.540	559.990
19	147.547	0.684	62	493.979	93.735	105	991.796	103.518
20	158.475	3.053	63	500.895	39.448	106	1002.588	3123.519
21	162.704	2.765	64	512.583	45.739	107	1008.412	733.346
22	169.403	0.264	65	532.133	35.621	108	1033.201	642.239
23	173.146	2.385	66	542.743	26.992	109	1041.204	193.140
24	174.844	0.565	67	569.910	32.157	110	1068.722	198.254
25	198.853	0.356	68	580.267	1.549	111	1070.868	683.826
26	203.936	3.550	69	590.630	24.903	112	1087.682	703.669
27	207.873	99.520	70	596.665	78.153	113	1097.531	285.750
28	218.657	8.753	71	606.610	41.136	114	1115.512	782.327
29	225.316	9.322	72	617.488	20.501	115	1128.417	1089.724
30	237.770	35.454	73	624.357	176.039	116	1298.057	119.743
31	248.042	77.209	74	635.051	41.891	117	1699.675	139.507
32	255.981	22.561	75	649.858	198.797	118	1720.126	115.958
33	261.064	2.932	76	655.555	162.835	119	1776.893	61.590
34	264.945	38.419	77	663.547	25.301	120	2317.110	144.674
35	270.890	4.501	78	680.982	63.395	121	2342.656	91.669
36	282.873	39.272	79	704.429	7.797	122	2489.422	2593.796
37	288.143	13.325	80	714.205	68.692	123	3449.633	696.921
38	292.182	10.271	81	719.046	89.091	124	3611.787	342.992
39	297.867	1.776	82	725.686	126.439	125	3745.560	225.242
40	298.809	12.941	83	733.257	58.751	126	3777.973	103.643
41	313.255	6.281	84	751.391	101.402	127	3845.709	59.961
42	317.807	48.939	85	776.353	56.308	128	3862.515	103.203

43	326.157	15.660	86	785.006	101.899	129	3865.063	100.014

Table 7 (6-6H_2O)
Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	25.826	1.195	36	245.077	5.432	71	530.126	22.428	106	944.950	88.933
2	30.048	0.045	37	248.482	8.913	72	540.864	17.948	107	950.115	34.110
3	47.010	6.655	38	259.192	23.273	73	559.020	107.277	108	960.001	151.364
4	52.052	3.173	39	267.719	22.749	74	582.550	11.214	109	975.976	48.682
5	57.329	4.390	40	273.023	5.944	75	584.791	2.883	110	997.032	592.755
6	60.749	7.512	41	275.445	4.233	76	590.962	27.238	111	1006.090	2459.615
7	64.292	0.549	42	293.175	0.892	77	600.671	42.670	112	1009.651	1397.497
8	68.882	3.847	43	296.451	7.530	78	606.323	49.500	113	1027.548	119.645
9	72.897	11.296	44	298.043	0.339	79	613.997	1.123	114	1038.107	1966.885
10	84.399	3.804	45	303.833	0.636	80	617.289	106.127	115	1040.241	65.072
11	89.173	12.362	46	316.805	25.632	81	639.610	64.688	116	1068.938	156.970
12	92.935	4.699	47	321.663	9.004	82	641.439	20.206	117	1098.591	32.459
13	95.580	4.008	48	326.733	18.071	83	670.469	212.044	118	1107.213	131.846
14	100.147	3.833	49	329.295	54.096	84	680.874	108.476	119	1123.091	5.473
15	102.361	1.495	50	337.573	38.836	85	685.657	99.910	120	1133.601	703.832
16	105.797	1.893	51	340.581	65.589	86	709.875	81.368	121	1141.367	457.371
17	106.287	0.139	52	348.938	150.115	87	716.890	67.029	122	1144.104	1827.440
18	123.537	0.398	53	352.564	93.464	88	720.560	7.369	123	1714.531	89.410
19	126.862	3.210	54	356.779	3.674	89	727.762	99.761	124	1740.635	79.257
20	134.241	1.270	55	359.316	6.475	90	737.471	65.015	125	1754.396	77.154
21	137.692	6.588	56	364.589	65.373	91	745.080	171.342	126	1773.720	88.133
22	141.200	0.318	57	374.847	75.457	92	764.821	162.215	127	2388.796	63.679
23	144.522	2.169	58	381.755	136.410	93	783.508	48.249	128	2389.397	79.516
24	149.677	1.590	59	402.812	43.425	94	796.203	133.215	129	3233.322	789.054
25	167.231	14.856	60	407.094	86.322	95	810.086	75.182	130	3586.772	563.926
26	173.455	39.407	61	414.113	32.626	96	818.952	275.795	131	3612.702	126.498
27	174.392	5.010	62	431.555	163.205	97	825.035	56.638	132	3655.774	207.096
28	177.625	18.065	63	444.482	34.517	98	850.027	274.396	133	3713.851	473.375
29	184.062	16.317	64	454.972	84.038	99	855.793	169.897	134	3794.945	182.030
30	195.356	4.257	65	465.089	21.199	100	860.339	262.144	135	3816.052	78.674
31	207.365	42.790	66	469.023	39.614	101	868.405	195.007	136	3843.881	49.909
32	210.080	23.721	67	478.955	1.662	102	885.211	4.264	137	3875.258	108.123
33	226.800	7.081	68	486.305	38.086	103	889.887	73.017	138	3878.367	99.963
34	235.336	7.070	69	504.224	61.238	104	917.227	145.040			
35	241.570	3.245	70	520.078	108.040	105	918.139	35.545			

Table 8 (7-1H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity
1	19.114	0.009	44	293.823	35.229	87	660.841	0.141
2	26.637	0.000	45	295.898	5.103	88	667.761	29.675
3	30.400	0.077	46	305.039	5.752	89	677.123	32.349
4	35.155	0.957	47	305.284	144.159	90	680.233	16.219
5	50.545	1.275	48	311.173	0.123	91	689.452	287.009
6	57.166	0.003	49	313.279	16.163	92	691.647	93.801
7	67.362	0.003	50	315.113	12.668	93	695.142	3.455
8	71.354	0.039	51	322.625	43.587	94	702.256	9.460
9	76.835	0.053	52	323.616	23.810	95	703.466	18.917
10	77.591	0.001	53	325.968	8.107	96	710.096	53.741
11	85.954	0.445	54	328.762	18.041	97	726.109	3.308
12	91.823	0.134	55	334.736	49.100	98	726.339	36.259
13	100.269	1.806	56	337.651	16.638	99	730.076	61.077
14	104.297	2.871	57	339.046	48.532	100	747.007	77.254
15	108.248	0.073	58	342.516	4.652	101	747.875	37.413
16	114.779	0.113	59	346.477	3.428	102	776.756	97.628
17	117.331	0.034	60	350.238	0.276	103	806.353	20.039
18	127.661	0.003	61	363.108	0.028	104	806.484	28.549
19	135.863	0.343	62	367.309	35.018	105	815.236	5.454
20	136.558	0.004	63	379.430	95.274	106	819.527	128.670
21	139.129	0.202	64	394.826	6.037	107	833.566	0.663
22	139.448	0.003	65	417.456	196.432	108	839.500	199.608
23	149.662	0.013	66	423.864	362.455	109	847.591	0.000
24	156.847	1.087	67	449.826	148.540	110	853.116	35.204
25	159.413	0.179	68	457.729	194.986	111	889.582	270.395
26	166.210	3.002	69	468.251	1.596	112	890.449	0.124
27	170.674	1.287	70	479.596	2.140	113	893.767	110.622
28	183.007	0.050	71	499.634	81.119	114	924.378	1989.196
29	198.819	2.029	72	505.284	5.475	115	925.787	0.911
30	206.615	0.746	73	524.529	5.374	116	928.380	990.109
31	209.946	0.200	74	546.624	0.452	117	941.556	1.008
32	225.980	0.220	75	570.734	7.113	118	943.048	1757.571
33	228.212	0.003	76	577.532	3.378	119	962.998	2910.004
34	235.056	6.160	77	579.610	19.814	120	965.508	367.988
35	235.313	0.603	78	581.107	22.290	121	967.193	0.981
36	254.741	1.663	79	608.584	6.668	122	983.908	1712.301
37	256.890	10.100	80	618.926	24.829	123	1026.244	25.817
38	265.932	0.056	81	622.133	3.180	124	1033.263	126.227
39	268.131	124.812	82	623.359	27.814	125	1035.207	18.861
40	279.767	0.185	83	629.483	36.943	126	1049.626	919.073

41	280.968	8.076	84	638.072	0.282	127	1720.236	34.932
42	285.038	6.342	85	653.120	169.295	128	3727.212	17.639
43	292.081	0.182	86	653.162	4.192	129	3818.448	227.902

Table 9 (8-2H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	12.287	0.327	36	233.555	1.883	71	477.717	4.810	106	825.082	109.136
2	15.605	0.026	37	247.695	7.125	72	479.339	1.179	107	843.571	0.261
3	23.256	0.019	38	248.525	2.972	73	531.514	26.176	108	852.289	16.132
4	40.067	0.262	39	265.450	6.211	74	559.010	26.150	109	852.588	27.750
5	47.593	0.002	40	266.300	4.302	75	559.046	48.093	110	853.663	25.317
6	47.926	0.510	41	270.298	5.815	76	572.804	2.051	111	874.693	54.658
7	49.689	0.289	42	271.315	1.766	77	575.173	1.306	112	876.141	210.655
8	67.502	0.023	43	283.550	7.457	78	577.413	7.063	113	893.429	108.737
9	70.905	0.090	44	284.340	24.990	79	580.209	8.887	114	898.611	167.598
10	79.221	0.751	45	286.351	7.378	80	589.648	27.570	115	900.000	245.679
11	85.522	0.700	46	287.963	2.714	81	608.448	5.641	116	938.425	147.953
12	91.949	22.465	47	295.472	0.585	82	609.157	0.124	117	940.119	101.741
13	95.288	0.246	48	297.630	1.938	83	613.564	3.591	118	944.518	3466.258
14	108.211	1.172	49	313.103	2.099	84	626.945	13.174	119	958.580	22.950
15	114.104	1.273	50	319.574	28.852	85	637.117	27.155	120	962.836	397.877
16	116.460	1.605	51	323.451	0.887	86	646.270	0.079	121	963.663	12.499
17	118.746	15.751	52	326.554	37.173	87	667.453	0.287	122	964.142	1.649
18	125.039	0.228	53	329.479	13.853	88	674.548	100.194	123	976.859	1647.236
19	127.032	0.623	54	333.312	106.441	89	674.628	2.514	124	985.332	698.787
20	131.218	26.912	55	334.623	83.143	90	675.757	131.825	125	992.493	11.527
21	132.244	0.683	56	337.735	96.375	91	682.341	21.619	126	994.899	1640.328
22	135.910	1.343	57	344.011	12.772	92	682.728	22.981	127	1018.373	812.355
23	141.062	3.774	58	346.426	0.484	93	693.894	308.337	128	1029.111	1560.875
24	144.411	27.976	59	350.268	148.716	94	698.756	234.312	129	1043.791	442.066
25	150.902	0.680	60	355.353	77.873	95	699.657	13.214	130	1051.011	60.469
26	154.124	6.733	61	357.917	10.572	96	707.896	35.357	131	1059.450	2.874
27	162.189	12.594	62	366.313	104.316	97	708.030	10.969	132	1069.980	483.760
28	162.902	6.636	63	379.918	243.522	98	718.174	27.966	133	1118.368	0.232
29	183.842	37.273	64	401.476	117.993	99	733.416	2.697	134	1124.629	1708.460
30	209.300	16.320	65	403.349	77.551	100	751.995	226.826	135	2344.613	11.261
31	216.716	9.720	66	424.890	199.330	101	755.947	44.261	136	2345.228	193.431
32	219.432	0.388	67	452.150	113.108	102	779.879	137.687	137	3886.248	14.802
33	219.620	2.567	68	454.967	124.849	103	816.848	70.597	138	3886.745	164.365
34	227.209	15.206	69	470.406	0.000	104	819.646	76.877			
35	228.307	1.354	70	475.664	60.279	105	821.258	51.656			

Table 10 (9-2H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

1	12.719	0.020	36	233.431	1.706	71	479.255	19.628	106	825.783	101.448
2	15.971	0.072	37	248.156	6.030	72	479.813	1.653	107	845.321	3.596
3	23.486	0.053	38	251.064	5.264	73	532.290	3.278	108	852.548	20.942
4	41.628	0.038	39	258.314	2.486	74	550.762	82.116	109	854.775	36.877
5	48.228	0.015	40	266.678	7.045	75	565.508	24.954	110	862.223	6.387
6	48.789	0.281	41	269.799	5.788	76	571.828	0.030	111	875.976	126.403
7	50.411	0.016	42	272.074	1.370	77	575.720	0.253	112	885.345	51.407
8	68.270	0.026	43	275.726	8.020	78	577.621	4.444	113	894.975	35.827
9	70.849	0.113	44	284.053	8.259	79	579.335	14.341	114	897.281	418.875
10	78.842	0.525	45	286.410	14.865	80	589.553	25.431	115	901.348	72.627
11	88.122	0.655	46	288.489	9.235	81	608.695	5.439	116	938.922	14.529
12	90.951	1.227	47	293.736	3.929	82	608.866	12.747	117	940.613	247.120
13	100.354	3.525	48	297.346	2.108	83	614.181	3.451	118	945.963	3312.331
14	106.836	8.600	49	313.710	3.449	84	625.414	13.347	119	957.182	18.773
15	113.005	1.359	50	320.157	33.561	85	638.679	22.272	120	960.665	235.036
16	115.636	11.159	51	323.191	0.423	86	645.880	1.828	121	962.407	209.260
17	121.177	35.727	52	327.347	1.433	87	667.243	8.138	122	964.001	24.918
18	123.402	9.128	53	329.602	11.887	88	670.885	13.666	123	978.103	1706.660
19	126.413	20.424	54	332.695	127.386	89	674.735	57.305	124	984.819	599.949
20	128.360	0.144	55	336.244	86.517	90	675.709	64.948	125	992.578	22.951
21	132.979	0.534	56	336.489	85.447	91	682.657	22.235	126	995.158	1786.487
22	136.944	7.292	57	344.077	4.136	92	683.033	27.189	127	1021.449	972.429
23	137.448	1.018	58	347.622	15.702	93	694.002	303.418	128	1035.492	885.053
24	145.310	8.984	59	349.809	153.145	94	699.187	220.055	129	1045.751	676.149
25	150.522	7.520	60	352.067	13.640	95	700.956	31.256	130	1052.986	127.522
26	153.447	10.890	61	357.431	36.586	96	704.222	10.237	131	1059.928	86.080
27	161.205	5.760	62	365.513	139.717	97	709.083	20.323	132	1068.999	407.197
28	163.891	8.913	63	383.192	238.777	98	718.371	26.274	133	1100.200	626.825
29	175.224	7.645	64	393.917	43.058	99	732.960	1.709	134	1120.697	1147.609
30	200.619	28.810	65	411.830	110.919	100	754.767	145.158	135	2336.294	108.384
31	218.116	5.919	66	422.081	213.893	101	764.938	88.736	136	2343.230	106.206
32	219.577	1.029	67	450.701	113.588	102	780.186	135.709	137	3883.944	90.078
33	223.179	15.535	68	454.934	125.902	103	807.484	359.802	138	3887.430	93.344
34	228.169	0.422	69	469.993	2.370	104	820.340	90.510			
35	229.635	18.628	70	476.212	66.140	105	823.890	51.781			

Table 11 (10-4H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	17.634	0.085	40	244.806	1.971	79	479.893	3.659	118	858.240	1.475
2	22.087	0.028	41	245.515	7.001	80	512.464	18.503	119	860.298	74.546
3	34.446	0.672	42	249.844	6.411	81	533.820	11.014	120	864.971	37.678
4	43.077	0.708	43	261.859	2.347	82	558.767	12.671	121	878.222	35.431
5	47.888	0.056	44	266.959	4.180	83	560.197	55.960	122	887.870	16.799
6	51.046	0.377	45	269.560	18.897	84	572.750	4.291	123	898.141	306.537
7	51.637	0.340	46	274.147	24.081	85	575.246	1.892	124	899.658	218.025
8	56.337	0.469	47	278.097	3.155	86	578.178	7.255	125	916.960	76.768
9	60.781	0.707	48	282.210	26.023	87	582.278	1.230	126	925.106	841.416
10	68.646	0.077	49	284.423	1.555	88	589.694	17.834	127	936.332	274.227
11	70.691	0.038	50	286.270	5.944	89	593.166	88.924	128	939.355	986.671
12	79.289	0.453	51	291.596	20.703	90	609.261	11.783	129	942.178	1367.007
13	79.899	0.804	52	294.298	6.090	91	610.189	8.062	130	955.077	66.850
14	93.369	0.320	53	305.531	15.978	92	613.500	3.532	131	963.223	31.092
15	98.926	0.164	54	314.775	8.330	93	627.076	2.456	132	972.909	874.620
16	110.579	4.465	55	321.456	12.150	94	634.650	14.069	133	980.244	1421.052
17	110.956	2.544	56	322.342	4.172	95	643.903	8.020	134	986.810	537.710
18	115.296	1.447	57	327.023	79.304	96	665.768	0.351	135	993.448	1062.728
19	116.923	1.766	58	329.866	14.857	97	674.139	14.705	136	1001.769	751.539
20	123.603	0.169	59	332.256	48.032	98	675.317	95.824	137	1018.508	1006.683
21	126.145	0.250	60	335.882	91.627	99	680.091	7.334	138	1029.973	1523.531
22	130.471	0.968	61	337.798	76.485	100	682.381	47.132	139	1036.209	140.377
23	136.072	0.978	62	342.116	36.887	101	684.360	29.180	140	1044.235	142.139
24	136.609	0.595	63	347.934	4.237	102	687.441	19.214	141	1050.387	334.503
25	137.787	0.443	64	349.318	86.353	103	694.036	245.788	142	1056.502	74.352
26	144.984	0.439	65	360.462	101.698	104	696.550	291.741	143	1066.140	444.649
27	155.143	0.962	66	361.436	29.975	105	701.243	100.911	144	1106.009	257.543
28	159.661	1.246	67	367.513	80.532	106	704.819	61.565	145	1117.436	1494.071
29	164.843	1.041	68	373.685	86.538	107	709.061	59.390	146	1148.669	85.537
30	167.182	0.106	69	399.595	102.502	108	713.385	81.134	147	1716.696	127.364
31	181.897	6.134	70	405.008	112.452	109	714.950	21.169	148	1745.675	46.234
32	195.484	1.407	71	421.395	99.805	110	726.017	15.080	149	2341.643	85.936
33	197.448	9.559	72	430.117	144.013	111	747.368	17.531	150	2346.322	108.759
34	208.986	3.376	73	451.303	99.210	112	748.510	191.160	151	3399.547	795.450
35	217.454	2.377	74	454.076	122.701	113	774.800	146.906	152	3542.335	508.614
36	222.642	0.290	75	462.065	138.046	114	818.057	123.163	153	3650.789	292.918
37	226.146	0.995	76	470.225	3.167	115	821.731	22.938	154	3704.695	91.847
38	232.240	1.435	77	472.945	36.029	116	846.665	9.948	155	3733.699	484.201
39	235.721	0.902	78	476.856	39.081	117	852.813	12.012	156	3862.590	74.876

Table 12 (11-5H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	18.588	0.178	43	233.230	2.196	85	548.922	60.400	127	882.545	80.244
2	22.303	0.036	44	244.401	4.310	86	559.834	15.108	128	887.368	26.847
3	27.076	0.039	45	247.160	1.331	87	563.319	67.087	129	897.343	346.681
4	40.645	0.449	46	255.378	3.144	88	573.317	5.891	130	899.489	200.958
5	47.643	0.034	47	264.970	4.157	89	575.817	3.613	131	923.954	756.942
6	49.580	0.659	48	268.151	3.185	90	579.221	4.822	132	933.896	221.955
7	52.174	0.226	49	271.719	6.410	91	582.919	8.585	133	941.784	1121.763
8	57.683	2.491	50	278.232	3.472	92	589.748	16.979	134	942.359	883.888
9	63.913	0.755	51	285.253	6.809	93	609.148	40.043	135	954.032	103.617
10	66.906	3.949	52	286.335	10.896	94	609.655	1.748	136	956.361	368.398
11	69.431	0.061	53	289.588	2.475	95	612.350	79.984	137	963.533	38.645
12	71.924	0.982	54	293.107	16.207	96	613.757	57.951	138	975.201	1327.333
13	79.279	0.243	55	294.320	3.946	97	627.934	12.470	139	984.214	689.752
14	86.052	8.495	56	314.794	7.270	98	632.548	48.417	140	988.555	697.332
15	93.279	0.342	57	318.537	5.564	99	634.040	7.321	141	995.862	1585.129
16	98.989	2.363	58	322.678	11.413	100	644.363	7.257	142	1006.226	444.553
17	111.017	4.791	59	323.728	1.229	101	665.122	0.324	143	1023.913	1060.968
18	113.501	1.565	60	327.519	69.635	102	674.149	69.965	144	1036.544	1496.204
19	115.090	4.020	61	331.137	13.049	103	676.403	74.756	145	1038.809	48.860
20	116.885	2.247	62	332.659	55.014	104	680.843	49.955	146	1046.706	252.898
21	125.741	1.063	63	336.640	99.145	105	682.722	30.932	147	1056.347	14.531
22	127.796	0.683	64	338.432	80.016	106	686.833	15.326	148	1066.375	437.458
23	132.770	3.329	65	342.537	29.501	107	687.674	4.560	149	1093.254	689.028
24	133.245	10.827	66	348.273	6.275	108	693.713	294.305	150	1118.230	1173.634
25	135.933	3.797	67	350.168	92.089	109	696.127	165.565	151	1172.911	160.752
26	137.024	0.038	68	361.098	21.558	110	700.817	82.814	152	1200.053	137.846
27	141.015	16.616	69	362.807	61.285	111	704.962	132.333	153	1710.172	86.932
28	148.186	1.744	70	368.709	80.746	112	708.391	85.607	154	1728.325	140.654
29	153.655	104.892	71	374.526	59.841	113	713.952	31.980	155	1797.870	81.314
30	157.397	6.109	72	396.444	205.196	114	724.129	28.932	156	2344.186	78.396
31	161.741	7.889	73	401.553	89.665	115	728.692	96.066	157	2347.886	105.329
32	165.910	1.132	74	408.445	42.721	116	740.833	189.606	158	3237.740	1231.058
33	168.574	11.386	75	422.535	96.383	117	746.936	71.363	159	3525.109	480.766
34	175.194	5.007	76	437.289	119.612	118	761.110	73.024	160	3592.936	311.497
35	188.793	7.048	77	451.399	93.080	119	774.213	134.975	161	3638.593	160.499
36	210.492	0.654	78	455.277	119.322	120	816.289	115.243	162	3652.474	498.739
37	214.524	2.210	79	469.431	4.487	121	822.931	35.648	163	3689.329	309.982
38	221.229	1.155	80	473.584	29.103	122	845.842	11.350	164	3758.850	291.342
39	223.670	2.517	81	475.684	45.648	123	851.645	9.641	165	3870.332	95.756
40	226.399	0.705	82	479.890	5.873	124	857.153	13.396			
41	230.465	3.920	83	507.660	19.302	125	859.385	66.511			
42	232.642	0.719	84	533.103	30.627	126	866.887	34.641			

Table 13 (12-7H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

1	14.478	0.576	47	244.786	3.322	93	562.397	49.154	139	897.189	337.837
2	19.865	0.211	48	253.167	3.824	94	573.764	3.852	140	899.171	101.373
3	22.774	0.659	49	254.729	0.083	95	578.940	0.763	141	920.987	1167.567
4	35.644	0.915	50	264.849	12.878	96	579.872	11.287	142	928.569	305.961
5	37.569	1.054	51	265.932	1.895	97	582.863	16.670	143	934.888	376.702
6	39.821	1.880	52	269.953	7.116	98	594.419	22.417	144	938.125	158.731
7	46.640	0.666	53	276.507	1.152	99	602.422	155.960	145	943.575	66.019
8	48.034	5.006	54	276.774	6.464	100	609.113	2.785	146	950.214	113.018
9	50.084	3.200	55	277.403	11.464	101	610.150	10.785	147	954.984	21.233
10	55.276	13.742	56	282.631	9.279	102	613.655	41.340	148	958.042	166.795
11	61.984	12.317	57	288.457	1.210	103	628.767	26.431	149	961.258	273.072
12	62.969	0.526	58	292.778	21.884	104	632.794	24.441	150	964.848	1121.638
13	71.535	1.140	59	293.573	8.050	105	634.787	13.712	151	969.515	21.694
14	78.831	24.494	60	295.633	20.859	106	650.574	3.966	152	983.122	518.061
15	85.994	0.056	61	299.159	116.067	107	670.327	19.387	153	991.431	598.400
16	87.479	5.849	62	318.922	14.309	108	674.521	204.879	154	998.496	1508.560
17	94.681	4.795	63	321.850	22.018	109	678.332	171.277	155	1006.135	165.484
18	102.089	4.158	64	324.049	5.560	110	685.090	16.155	156	1025.110	1041.029
19	104.899	37.781	65	324.947	24.980	111	686.775	18.889	157	1027.274	1710.197
20	108.312	13.527	66	332.392	45.129	112	688.245	143.770	158	1037.349	1770.291
21	111.523	1.670	67	335.496	67.993	113	692.707	30.079	159	1057.158	204.336
22	117.175	3.867	68	336.221	47.730	114	695.906	32.854	160	1062.073	106.681
23	119.862	18.940	69	341.861	16.130	115	699.987	53.783	161	1068.416	119.634
24	124.692	0.967	70	349.072	0.827	116	704.981	103.588	162	1070.304	244.792
25	126.814	4.475	71	357.352	19.242	117	708.754	53.547	163	1092.945	650.261
26	128.063	2.755	72	359.932	84.725	118	713.702	11.330	164	1117.794	1147.864
27	132.405	0.240	73	363.437	6.612	119	717.976	93.061	165	1164.097	143.397
28	136.580	3.275	74	364.424	43.793	120	721.713	71.063	166	1201.238	134.983
29	141.378	8.868	75	373.352	44.600	121	725.715	84.513	167	1709.303	86.311
30	143.566	9.559	76	389.486	244.760	122	739.713	190.747	168	1727.922	144.881
31	147.694	12.273	77	393.192	101.860	123	747.018	84.635	169	1797.485	82.974
32	150.876	6.872	78	404.770	85.695	124	759.705	99.305	170	2344.641	73.365
33	159.510	6.783	79	408.044	63.222	125	767.532	242.787	171	2347.400	108.345
34	165.681	12.710	80	416.456	90.295	126	777.649	90.587	172	2353.802	115.551
35	174.644	1.213	81	424.397	76.517	127	791.333	105.019	173	2356.164	76.751
36	177.920	81.289	82	434.484	87.052	128	816.516	127.642	174	3233.514	1258.004
37	184.059	6.419	83	448.488	207.118	129	822.618	33.544	175	3532.446	472.483
38	206.822	4.873	84	454.975	128.350	130	823.268	26.913	176	3594.070	308.225
39	209.954	5.756	85	470.336	9.825	131	829.188	63.970	177	3637.582	146.230
40	212.899	12.991	86	473.842	48.624	132	855.662	15.725	178	3651.489	527.798
41	215.709	1.831	87	475.512	59.665	133	859.346	64.335	179	3686.846	299.088

42	222.036	2.277	88	480.833	5.548	134	867.387	27.558	180	3757.790	302.148
43	225.556	2.693	89	502.174	15.995	135	880.860	97.228	181	3870.057	95.725
44	227.343	0.899	90	529.052	35.197	136	882.342	50.107	182	3875.616	46.512
45	229.835	3.540	91	547.944	88.749	137	883.237	211.027	183	3877.880	86.224
46	242.942	1.068	92	560.390	80.112	138	890.084	539.409			

Table 14 (13-11H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	16.664	2.302	56	269.470	2.824	111	607.744	127.007	166	946.161	51.305
2	18.578	0.083	57	270.456	5.270	112	619.166	39.429	167	950.838	90.323
3	22.041	1.757	58	274.258	0.294	113	623.910	90.007	168	952.158	46.491
4	23.755	0.172	59	279.798	1.440	114	630.144	13.441	169	955.103	341.385
5	38.285	0.730	60	281.792	7.119	115	633.737	4.223	170	958.183	26.817
6	43.412	0.392	61	285.648	1.273	116	640.914	25.386	171	963.722	127.559
7	46.992	1.163	62	287.808	6.521	117	653.182	39.453	172	964.678	373.744
8	50.154	1.478	63	291.962	1.214	118	666.679	123.483	173	968.890	56.085
9	55.979	10.592	64	299.197	7.959	119	674.582	82.933	174	970.961	70.669
10	57.162	0.516	65	300.641	4.483	120	685.268	128.265	175	974.555	1100.817
11	67.953	1.777	66	305.624	2.257	121	686.726	26.345	176	981.131	110.226
12	72.613	6.426	67	307.173	49.734	122	689.407	43.595	177	988.235	46.303
13	75.317	0.782	68	308.972	4.395	123	692.850	0.252	178	1005.555	939.126
14	77.134	7.842	69	320.123	96.398	124	696.229	4.138	179	1010.846	1436.498
15	82.437	0.394	70	325.235	10.476	125	698.843	54.486	180	1027.214	504.938
16	85.774	4.675	71	327.409	12.276	126	703.737	10.161	181	1034.849	173.474
17	88.760	0.867	72	335.178	97.739	127	705.627	8.016	182	1037.527	1393.902
18	97.654	4.318	73	337.266	10.004	128	711.495	9.385	183	1050.453	164.323
19	98.607	2.261	74	341.649	20.202	129	713.833	9.382	184	1059.667	41.571
20	102.467	1.326	75	344.421	15.089	130	716.021	44.213	185	1064.939	450.342
21	109.272	2.524	76	350.652	51.219	131	717.894	74.906	186	1071.748	1308.561
22	110.493	3.226	77	355.630	1.214	132	721.955	111.243	187	1074.925	131.207
23	114.430	12.266	78	359.586	32.492	133	726.766	27.718	188	1077.731	210.931
24	117.671	2.333	79	362.243	17.197	134	738.770	108.936	189	1081.955	949.248
25	123.856	4.187	80	365.366	10.553	135	741.037	182.486	190	1089.168	402.697
26	127.619	6.784	81	376.297	2.491	136	742.982	72.180	191	1108.876	649.156
27	129.465	4.749	82	384.376	67.208	137	752.122	107.254	192	1136.020	1134.562
28	130.647	1.112	83	392.473	51.656	138	768.248	194.785	193	1148.766	140.716
29	134.874	19.637	84	396.162	367.052	139	786.528	105.543	194	1207.228	127.176
30	138.679	2.110	85	406.451	103.036	140	789.065	32.781	195	1710.661	85.685
31	140.690	10.971	86	408.292	47.657	141	794.667	48.033	196	1730.268	145.280
32	145.837	11.311	87	409.920	52.445	142	799.316	109.399	197	1799.025	76.705
33	147.772	106.558	88	421.943	195.838	143	818.504	10.009	198	2316.699	108.027
34	151.320	62.390	89	431.739	17.600	144	825.232	75.155	199	2319.611	170.341
35	156.442	98.914	90	437.742	99.198	145	826.999	54.808	200	2322.401	123.668

36	166.856	3.483	91	441.858	9.397	146	836.556	51.037	201	2347.298	103.493
37	183.033	5.111	92	443.663	70.458	147	842.101	62.059	202	2352.512	99.804
38	186.972	48.284	93	450.748	256.891	148	846.951	146.151	203	2355.533	119.054
39	194.379	10.755	94	455.660	74.952	149	848.526	17.048	204	2358.905	132.986
40	196.926	10.109	95	464.579	10.217	150	853.026	33.782	205	2360.317	90.980
41	200.619	3.252	96	471.767	94.323	151	857.242	39.822	206	3233.861	1319.205
42	203.668	15.057	97	477.304	58.476	152	860.175	48.970	207	3582.448	258.556
43	209.505	6.176	98	479.546	9.116	153	864.373	57.937	208	3599.546	394.163
44	212.966	3.485	99	494.494	6.540	154	868.113	170.116	209	3634.389	479.662
45	215.385	12.410	100	530.580	33.435	155	884.023	527.560	210	3639.085	527.296
46	219.838	15.621	101	544.508	42.034	156	886.677	502.736	211	3640.201	142.209
47	220.138	4.162	102	554.726	18.073	157	888.250	116.338	212	3659.135	601.390
48	229.657	18.819	103	555.935	37.240	158	889.625	203.754	213	3691.593	215.686
49	231.773	13.516	104	574.920	0.518	159	911.636	303.784	214	3753.833	356.201
50	236.288	17.099	105	576.895	12.635	160	924.518	173.854	215	3853.870	100.557
51	246.708	5.389	106	581.445	14.975	161	931.606	1346.735	216	3855.911	70.974
52	252.208	9.671	107	586.923	9.366	162	938.447	49.142	217	3860.716	106.167
53	255.300	2.913	108	589.084	116.550	163	940.286	83.935	218	3867.081	93.215
54	258.394	4.413	109	595.088	194.017	164	943.938	226.076	219	3877.508	105.535
55	262.567	16.609	110	600.781	66.729	165	945.075	261.592			

Table 15 (14-1H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	8.958	0.010	37	258.305	14.203	73	481.254	2.033	109	813.953	110.684
2	13.019	0.005	38	259.482	6.454	74	504.212	102.353	110	821.710	42.019
3	23.780	0.341	39	269.028	2.064	75	514.779	1.202	111	829.180	0.796
4	30.247	2.169	40	271.004	102.519	76	517.605	0.008	112	830.251	98.746
5	34.809	4.387	41	271.636	3.574	77	523.715	48.745	113	847.486	178.201
6	54.219	0.049	42	272.025	5.318	78	538.672	20.765	114	850.254	7.981
7	70.942	1.672	43	278.909	0.519	79	550.221	251.702	115	866.167	0.260
8	75.487	0.517	44	279.283	0.529	80	567.710	252.565	116	869.329	210.115
9	76.884	0.270	45	291.248	20.589	81	588.984	220.678	117	873.343	154.890
10	92.633	1.044	46	297.086	8.981	82	597.226	0.389	118	898.741	365.210
11	93.149	0.447	47	299.513	10.437	83	604.122	77.951	119	901.900	181.676
12	101.385	19.411	48	299.908	20.775	84	612.644	36.286	120	932.111	405.738
13	103.661	0.432	49	304.527	18.655	85	616.663	24.853	121	938.828	35.763
14	107.808	9.775	50	307.027	99.452	86	618.916	4.846	122	945.111	102.011
15	108.705	5.366	51	313.886	9.033	87	624.208	3.876	123	955.038	1.309
16	115.980	0.059	52	314.795	52.342	88	635.920	0.922	124	963.701	1142.321
17	122.404	29.323	53	322.583	115.199	89	639.543	235.902	125	964.296	29.933
18	125.646	35.131	54	324.852	17.808	90	653.539	11.316	126	967.931	288.450
19	132.874	0.326	55	328.964	0.063	91	654.013	238.954	127	976.440	543.304

20	135.069	0.204	56	330.323	9.134	92	655.822	38.674	128	980.768	2982.513
21	142.377	1.671	57	341.263	2.435	93	702.433	2.369	129	1002.082	2321.682
22	153.875	8.322	58	343.040	0.051	94	707.286	10.253	130	1007.594	309.002
23	160.349	6.147	59	352.520	203.248	95	712.217	3.406	131	1008.444	117.194
24	160.746	4.011	60	355.915	7.864	96	713.341	9.173	132	1059.936	270.051
25	166.041	34.290	61	356.238	42.856	97	715.794	1.686	133	1077.519	682.009
26	167.301	0.539	62	360.487	13.930	98	720.573	85.900	134	1093.089	19.536
27	172.888	0.344	63	373.900	29.645	99	731.367	24.904	135	1094.636	645.242
28	189.110	0.537	64	376.507	2.731	100	733.029	33.679	136	1098.653	21.508
29	194.700	1.682	65	377.094	4.935	101	750.902	94.247	137	1115.672	931.278
30	208.485	157.986	66	389.881	189.100	102	763.837	19.419	138	1127.819	142.799
31	209.183	2.429	67	402.534	37.058	103	773.002	52.067	139	1144.658	1035.342
32	211.308	5.346	68	404.977	0.247	104	775.790	142.385	140	2128.791	213.007
33	217.406	1.273	69	417.917	196.793	105	785.881	78.292	141	3855.293	191.412
34	226.952	2.214	70	460.221	2.717	106	790.483	227.058			
35	229.203	15.214	71	463.167	6.785	107	791.398	20.446			
36	244.532	1.777	72	473.089	77.768	108	796.357	0.339			

Table 16 (15-6H_2O)
Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	15.835	0.367	48	250.763	0.831	95	507.781	12.651	142	913.448	130.824
2	23.852	0.382	49	254.614	3.365	96	520.764	10.909	143	921.612	312.701
3	27.535	0.568	50	263.586	3.886	97	528.820	141.368	144	927.315	7.148
4	29.180	2.084	51	266.452	6.287	98	531.149	51.673	145	935.405	16.080
5	35.226	1.200	52	270.927	7.781	99	538.122	8.653	146	947.663	61.262
6	39.813	2.340	53	274.953	12.515	100	540.305	82.310	147	953.900	31.980
7	48.273	0.710	54	279.874	3.375	101	568.115	60.873	148	970.636	77.890
8	54.851	4.626	55	284.799	6.183	102	577.445	52.112	149	981.830	20.575
9	58.430	7.384	56	286.405	15.844	103	584.165	9.525	150	999.010	1528.733
10	62.711	1.905	57	290.039	12.488	104	585.209	0.610	151	1003.829	854.661
11	64.635	1.239	58	291.804	6.383	105	586.300	16.122	152	1010.104	250.613
12	68.626	0.425	59	293.184	29.488	106	590.653	83.577	153	1016.290	1700.853
13	73.631	2.998	60	300.215	83.081	107	603.140	13.985	154	1018.458	421.775
14	76.950	0.200	61	303.860	146.966	108	607.459	80.063	155	1020.713	2250.034
15	83.034	2.041	62	306.696	6.588	109	613.592	95.465	156	1032.041	91.087
16	88.856	0.625	63	319.812	31.796	110	615.352	164.230	157	1032.957	1822.469
17	91.652	8.970	64	321.081	82.152	111	618.839	178.046	158	1042.756	940.885
18	98.170	0.629	65	323.126	3.695	112	629.776	38.882	159	1069.273	421.199
19	102.027	1.023	66	325.781	3.567	113	642.133	74.433	160	1073.094	449.151
20	110.084	0.167	67	329.177	0.719	114	653.256	3.553	161	1078.692	79.867
21	111.067	3.969	68	332.636	1.598	115	685.649	54.520	162	1085.977	259.752
22	115.946	2.472	69	335.845	16.704	116	693.679	107.003	163	1094.025	100.571

23	120.268	0.264	70	343.218	22.324	117	700.711	14.131	164	1096.770	4.980
24	121.523	0.521	71	346.761	19.349	118	716.066	11.966	165	1111.761	661.109
25	125.701	0.555	72	348.491	173.595	119	716.832	90.956	166	1117.910	505.528
26	130.410	5.869	73	352.242	202.749	120	720.022	27.514	167	1131.344	1174.645
27	134.297	5.114	74	354.586	17.947	121	723.055	80.771	168	1135.269	505.288
28	137.434	8.001	75	358.312	32.033	122	728.875	70.361	169	1145.297	1077.685
29	143.810	4.073	76	360.096	14.674	123	734.832	42.141	170	1153.894	715.324
30	149.808	1.395	77	365.531	94.866	124	739.344	77.300	171	1720.257	91.324
31	154.804	8.898	78	366.960	27.860	125	763.094	40.511	172	1739.736	123.405
32	160.990	2.449	79	369.879	21.489	126	770.562	126.187	173	1750.980	86.361
33	167.704	1.485	80	380.402	86.669	127	775.342	11.542	174	1769.523	107.686
34	170.528	0.102	81	391.968	18.532	128	794.820	87.418	175	2332.097	89.553
35	174.750	3.375	82	395.358	32.833	129	799.109	16.874	176	2347.785	95.210
36	176.346	12.054	83	406.993	4.855	130	816.936	29.467	177	2986.634	1479.662
37	184.685	0.784	84	410.066	42.800	131	819.502	176.805	178	3356.979	771.835
38	186.495	6.701	85	424.465	28.593	132	824.055	166.436	179	3464.813	681.026
39	192.455	13.190	86	428.304	52.998	133	838.092	255.146	180	3657.348	120.318
40	194.282	12.765	87	432.430	107.721	134	844.648	170.246	181	3679.561	208.187
41	206.335	10.612	88	450.895	17.783	135	862.771	230.998	182	3740.819	470.001
42	213.078	7.760	89	462.026	61.087	136	874.277	85.780	183	3816.688	79.569
43	219.155	14.054	90	471.088	12.618	137	883.570	174.290	184	3842.193	86.306
44	223.652	19.672	91	478.082	41.960	138	890.888	5.014	185	3855.849	48.854
45	224.896	35.045	92	480.516	0.984	139	896.591	15.475	186	3876.802	124.403
46	239.159	9.540	93	490.431	7.437	140	901.162	35.893			
47	246.022	0.868	94	498.468	128.447	141	904.782	160.370			

Table 17 (16-12H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	19.252	1.069	61	248.970	12.311	121	556.759	5.396	181	992.704	2467.725
2	25.433	0.462	62	254.002	1.646	122	562.950	83.525	182	1005.695	53.071
3	29.425	0.266	63	261.501	23.135	123	570.114	20.657	183	1013.844	988.860
4	33.114	1.282	64	267.905	57.805	124	572.374	86.607	184	1018.346	784.098
5	37.791	0.233	65	270.462	36.653	125	581.729	1.096	185	1021.736	1304.540
6	42.575	0.275	66	272.978	1.987	126	586.369	87.160	186	1028.851	306.389
7	44.209	0.156	67	276.523	4.447	127	588.264	36.783	187	1033.833	847.956
8	48.718	0.668	68	277.986	4.328	128	598.994	36.268	188	1035.661	43.025
9	49.866	0.854	69	282.142	15.061	129	603.736	63.566	189	1040.573	2047.804
10	54.760	2.240	70	284.012	17.864	130	605.235	30.631	190	1049.762	463.491
11	57.805	1.192	71	285.425	18.598	131	608.008	38.478	191	1064.724	11.956
12	60.549	3.424	72	288.963	20.353	132	612.538	43.760	192	1071.931	79.861
13	64.929	2.699	73	293.807	1.005	133	614.272	48.126	193	1087.666	10.807
14	66.758	0.636	74	297.534	18.178	134	618.059	78.967	194	1092.032	100.182
15	70.261	1.194	75	299.589	6.995	135	636.793	3.148	195	1098.071	117.701

16	77.431	0.366	76	303.306	38.946	136	639.815	116.404	196	1109.257	319.881
17	78.646	0.100	77	308.727	5.846	137	646.451	39.889	197	1118.507	706.277
18	85.089	0.469	78	313.845	12.306	138	651.461	8.020	198	1121.687	209.881
19	87.580	1.082	79	318.444	15.448	139	663.464	18.216	199	1124.703	901.598
20	90.925	1.093	80	321.153	2.169	140	672.600	76.337	200	1138.158	611.966
21	93.382	0.783	81	325.820	12.207	141	682.588	219.405	201	1146.509	1101.436
22	99.351	2.934	82	327.587	19.264	142	698.112	24.563	202	1148.530	566.211
23	99.541	1.324	83	331.728	13.107	143	706.692	41.433	203	1192.748	245.748
24	106.199	0.850	84	338.861	13.812	144	711.107	16.632	204	1300.963	39.664
25	108.011	3.118	85	341.539	19.592	145	715.628	242.809	205	1334.075	211.569
26	113.044	0.863	86	344.110	36.468	146	718.266	56.686	206	1698.602	17.109
27	113.487	0.720	87	347.725	100.924	147	719.842	11.672	207	1709.518	129.444
28	116.433	1.717	88	349.353	182.516	148	724.182	15.561	208	1720.163	125.371
29	117.962	0.731	89	351.362	101.308	149	728.327	68.114	209	1733.580	100.559
30	122.725	7.718	90	353.913	71.173	150	731.798	34.934	210	1738.474	190.031
31	124.349	0.858	91	356.004	30.222	151	735.202	15.211	211	1748.271	316.444
32	126.129	2.308	92	357.878	18.248	152	748.856	169.650	212	1781.545	210.440
33	128.973	1.050	93	360.313	32.517	153	759.854	576.237	213	1784.925	23.842
34	131.542	1.714	94	364.925	91.357	154	764.288	83.177	214	1792.230	0.168
35	137.817	2.370	95	366.396	67.899	155	765.898	66.480	215	1815.595	166.950
36	138.769	1.135	96	372.044	49.456	156	773.239	82.023	216	1830.951	109.578
37	141.214	0.764	97	379.076	59.980	157	780.897	107.256	217	1978.840	2404.065
38	147.093	0.380	98	384.276	144.567	158	792.854	204.685	218	2372.593	61.254
39	149.389	2.365	99	387.215	72.695	159	796.523	178.942	219	2413.988	2769.108
40	159.065	3.215	100	400.377	22.885	160	807.879	31.457	220	3028.190	437.319
41	160.673	0.330	101	404.616	57.702	161	809.581	216.497	221	3047.252	1628.965
42	162.488	0.913	102	414.058	51.847	162	818.357	155.721	222	3272.128	700.961
43	163.116	0.366	103	419.674	147.475	163	822.773	53.994	223	3296.639	842.834
44	169.662	7.221	104	427.975	87.459	164	831.520	163.264	224	3390.398	498.250
45	171.806	2.892	105	436.230	95.999	165	853.303	49.810	225	3424.781	880.549
46	173.379	6.026	106	449.855	28.055	166	857.106	53.262	226	3477.141	617.141
47	176.248	0.336	107	458.631	14.184	167	863.337	97.940	227	3514.217	156.062
48	179.547	1.893	108	460.356	16.686	168	887.926	11.739	228	3522.534	1222.577
49	192.481	9.849	109	462.779	51.937	169	890.140	76.938	229	3560.640	436.629
50	193.642	6.485	110	468.022	56.037	170	893.973	42.843	230	3577.869	314.147
51	195.172	5.075	111	474.130	58.686	171	894.722	5.879	231	3590.922	102.116
52	200.563	4.307	112	481.420	7.621	172	899.680	48.846	232	3627.118	284.745
53	204.519	14.257	113	486.592	79.239	173	914.083	170.788	233	3665.414	468.313
54	209.318	12.285	114	487.517	32.707	174	922.255	396.107	234	3679.100	374.674
55	212.567	2.842	115	499.525	50.188	175	948.284	435.906	235	3707.160	229.694
56	219.154	1.688	116	516.191	10.898	176	949.186	26.013	236	3735.944	288.264
57	228.036	5.797	117	525.419	31.851	177	962.546	104.243	237	3812.344	158.745
58	232.059	59.823	118	532.943	65.255	178	972.089	217.320	238	3814.893	62.386
59	243.148	16.129	119	537.539	30.725	179	980.972	1402.402	239	3845.837	69.132
60	245.209	5.448	120	542.044	85.696	180	984.576	87.936	240	3869.027	70.742

Table 18 (17-1H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	34.621	7.255	38	249.329	2.013	75	457.011	3.901	112	824.456	117.814
2	46.638	2.365	39	250.779	10.681	76	486.186	3.982	113	827.418	139.746
3	66.386	0.010	40	252.039	22.923	77	487.478	8.388	114	866.477	1.739
4	69.008	6.824	41	262.401	355.791	78	492.635	13.408	115	879.424	2.933
5	70.167	1.319	42	265.400	6.883	79	500.179	0.840	116	894.465	2.868
6	73.839	0.263	43	268.660	1.237	80	506.503	118.417	117	895.284	0.028
7	77.628	0.091	44	271.994	6.073	81	507.132	118.367	118	902.956	49.269
8	78.768	0.781	45	272.610	0.153	82	531.299	0.217	119	911.712	178.423
9	81.096	1.305	46	277.002	9.253	83	533.602	67.682	120	922.700	87.701
10	84.189	0.860	47	280.363	8.834	84	540.248	193.546	121	981.413	3.183
11	94.773	1.612	48	282.018	5.297	85	579.497	12.149	122	989.325	4.602
12	104.728	20.464	49	291.260	26.362	86	584.703	2.756	123	989.942	0.301
13	109.650	2.074	50	302.370	8.318	87	585.915	0.260	124	990.848	1.474
14	109.944	0.049	51	319.124	0.067	88	602.182	7.896	125	992.382	0.985
15	120.623	0.775	52	320.895	3.874	89	607.006	0.385	126	993.683	13.021
16	123.873	0.041	53	333.764	10.550	90	610.211	113.527	127	994.013	1.871
17	124.665	0.337	54	333.822	1.340	91	629.866	237.328	128	999.133	6.793
18	130.747	0.270	55	338.431	173.521	92	630.391	266.774	129	1000.576	15.522
19	135.494	0.622	56	343.368	136.235	93	632.515	4.500	130	1016.034	2728.285
20	138.401	4.022	57	350.737	181.734	94	643.085	2.080	131	1016.097	2693.850
21	143.811	10.871	58	352.008	64.472	95	654.312	0.592	132	1017.511	2713.179
22	161.792	3.678	59	353.982	47.983	96	655.862	0.651	133	1059.799	0.045
23	162.191	2.726	60	354.540	35.029	97	705.344	91.446	134	1062.164	3.042
24	169.234	4.510	61	358.279	31.503	98	709.992	34.126	135	1078.911	0.317
25	174.507	0.356	62	359.759	70.868	99	715.389	8.027	136	1086.094	56.198
26	176.425	0.188	63	360.236	1.121	100	719.176	32.328	137	1087.695	2.835
27	176.870	0.039	64	372.011	5.570	101	721.387	63.966	138	1099.213	2183.463
28	181.569	1.734	65	373.280	0.397	102	725.942	119.996	139	1100.505	1423.959
29	182.721	1.023	66	374.322	0.940	103	727.252	48.441	140	1104.351	0.938
30	191.233	0.415	67	390.328	15.822	104	727.629	2.670	141	1106.706	871.769
31	194.116	0.326	68	394.084	0.091	105	737.829	136.968	142	1108.140	322.548
32	206.996	2.412	69	394.422	0.029	106	763.198	4.150	143	1110.278	213.190
33	209.369	0.369	70	398.862	9.329	107	763.618	0.122	144	1119.347	2413.094
34	211.021	0.088	71	416.675	0.102	108	804.704	0.440	145	1681.416	70.602
35	224.413	1.255	72	419.599	7.272	109	805.666	0.173	146	3743.829	7.533
36	233.295	16.686	73	450.571	54.277	110	812.412	382.333	147	3863.095	74.716
37	246.755	14.756	74	451.652	44.077	111	812.437	368.192			

Table 19 (18-4H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	28.920	0.239	51	242.661	0.703	101	494.735	0.262	151	850.244	2.051
2	32.873	1.243	52	245.320	1.094	102	512.561	0.749	152	851.183	77.190
3	34.957	0.535	53	247.864	0.099	103	541.541	4.447	153	851.441	48.402
4	38.246	0.231	54	262.470	1.476	104	569.276	5.278	154	852.524	29.545
5	46.489	0.233	55	264.247	2.947	105	575.168	2.489	155	854.538	66.496
6	51.012	0.242	56	268.151	3.617	106	575.257	0.854	156	856.098	161.575
7	57.376	0.261	57	269.024	8.543	107	578.440	0.284	157	856.811	188.591
8	63.669	0.066	58	271.070	0.933	108	580.058	0.682	158	887.351	396.694
9	67.525	0.185	59	276.749	11.782	109	580.411	0.041	159	902.439	0.481
10	68.913	0.089	60	281.538	4.168	110	589.166	10.616	160	910.199	6.053
11	72.530	0.009	61	282.450	9.602	111	599.934	35.886	161	911.705	2.761
12	73.107	0.029	62	282.898	0.400	112	623.657	90.551	162	914.588	0.282
13	90.713	0.336	63	284.254	22.846	113	624.378	45.646	163	924.842	6.321
14	91.485	3.987	64	288.686	20.024	114	625.562	1.090	164	937.969	45.695
15	93.985	2.044	65	294.496	10.345	115	640.999	1.233	165	939.428	52.209
16	104.314	1.060	66	296.356	4.232	116	642.655	6.026	166	940.199	2.962
17	107.056	0.857	67	301.928	48.131	117	643.938	10.067	167	940.257	29.078
18	107.469	1.471	68	312.055	19.309	118	659.534	0.544	168	945.360	375.230
19	115.836	13.096	69	312.652	4.924	119	674.061	204.248	169	953.494	103.941
20	120.810	3.305	70	313.307	25.601	120	675.901	1.051	170	954.478	4.926
21	122.934	2.750	71	321.836	2.789	121	677.530	135.633	171	956.591	65.572
22	125.514	1.243	72	325.308	52.496	122	680.514	47.634	172	958.628	103.933
23	126.734	0.063	73	325.571	82.942	123	683.243	2.885	173	964.485	178.262
24	129.549	3.530	74	327.786	127.533	124	689.366	8.410	174	967.375	28.318
25	130.606	6.273	75	328.675	12.832	125	690.262	3.238	175	968.961	32.016
26	132.610	3.473	76	331.040	15.116	126	697.530	1.101	176	977.494	2626.036
27	133.760	3.849	77	337.260	5.232	127	699.183	8.809	177	978.118	2656.968
28	136.400	1.168	78	340.541	1.575	128	707.498	2.708	178	982.598	1750.280
29	137.975	0.305	79	343.521	1.104	129	708.110	12.608	179	985.923	113.325
30	147.976	139.366	80	352.978	1.896	130	709.408	2.379	180	1012.377	2142.935
31	149.224	40.801	81	353.256	2.239	131	713.369	149.483	181	1014.221	2226.526
32	150.998	84.641	82	353.624	0.771	132	713.761	107.871	182	1029.377	3565.514
33	155.420	25.371	83	357.865	3.116	133	715.771	3.768	183	1057.928	21.280
34	159.037	11.953	84	363.992	7.194	134	720.784	7.382	184	1058.807	135.219
35	159.847	15.162	85	364.902	12.708	135	724.086	10.651	185	1062.092	349.897
36	163.974	30.003	86	366.464	11.224	136	724.421	3.133	186	1063.860	32.981
37	164.818	13.368	87	380.647	48.595	137	725.199	37.742	187	1065.330	53.277
38	173.518	2.620	88	386.339	132.685	138	731.002	480.407	188	1070.139	398.029
39	184.189	13.483	89	395.195	316.710	139	731.909	12.925	189	1071.942	734.196
40	185.258	7.516	90	409.617	41.946	140	734.619	3.406	190	1078.855	0.205
41	186.852	11.528	91	418.195	159.483	141	735.270	235.947	191	2312.173	225.940
42	189.054	19.405	92	444.175	548.558	142	773.443	235.680	192	2312.372	65.338
43	199.029	15.088	93	445.321	555.598	143	775.304	223.266	193	2312.821	113.921

44	201.090	0.916	94	459.895	55.962	144	775.649	261.680	194	2351.576	101.179
45	205.860	4.445	95	474.040	17.846	145	786.871	1.229	195	3870.657	66.231
46	214.417	0.232	96	475.891	10.453	146	794.386	94.794	196	3879.350	128.900
47	216.103	11.673	97	479.774	0.616	147	829.179	52.980	197	3879.616	62.694
48	217.452	0.312	98	481.797	0.367	148	848.663	91.822	198	3880.016	109.434
49	223.038	6.423	99	484.591	6.062	149	849.074	46.248			
50	223.652	0.085	100	485.196	10.913	150	849.707	11.060			

Table 20 (19-9H_2O)

Freq-Frequency (cm^{-1}), Intensity (km/mol)

	Freq	Intensity		Freq	Intensity		Freq	Intensity		Freq	Intensity
1	14.256	1.070	65	260.064	7.027	129	538.250	256.000	193	922.336	358.252
2	23.256	0.211	66	261.936	2.354	130	540.125	24.447	194	935.196	125.914
3	30.728	0.341	67	269.602	27.981	131	546.888	161.789	195	938.684	146.128
4	31.459	1.486	68	274.188	4.651	132	548.802	10.086	196	940.339	49.370
5	41.368	0.720	69	276.383	8.912	133	583.940	5.003	197	944.155	48.192
6	46.005	1.032	70	279.924	10.568	134	586.322	9.169	198	946.927	143.308
7	50.665	1.387	71	282.220	16.185	135	587.031	18.920	199	956.373	49.528
8	62.132	0.415	72	286.724	5.018	136	590.616	6.421	200	957.887	49.062
9	64.388	0.055	73	287.520	10.277	137	605.581	43.674	201	959.040	385.192
10	68.429	0.372	74	289.569	11.082	138	609.647	47.587	202	964.850	106.323
11	71.303	0.334	75	291.683	12.488	139	611.791	33.420	203	968.810	79.814
12	73.239	2.046	76	292.641	3.655	140	613.790	7.646	204	973.711	93.763
13	77.093	0.577	77	295.526	6.821	141	616.290	94.888	205	980.221	158.071
14	81.017	2.128	78	297.937	8.598	142	621.718	86.581	206	984.889	411.656
15	83.043	0.218	79	302.215	18.121	143	626.651	78.063	207	991.319	989.718
16	84.952	4.557	80	305.519	5.695	144	635.031	118.616	208	1008.126	104.864
17	89.471	0.057	81	306.255	8.828	145	644.636	89.107	209	1014.939	770.367
18	91.551	0.657	82	309.049	2.469	146	647.054	48.653	210	1018.556	676.914
19	95.604	3.710	83	312.576	36.240	147	654.336	97.494	211	1019.861	2535.049
20	97.864	1.900	84	315.972	12.074	148	656.441	6.571	212	1021.231	1608.083
21	104.313	0.936	85	319.847	14.242	149	673.132	177.933	213	1026.678	2390.609
22	107.344	3.661	86	322.680	1.894	150	675.359	68.264	214	1031.418	398.317
23	109.236	1.837	87	326.967	7.720	151	712.503	2.227	215	1032.017	737.409
24	111.545	0.976	88	327.529	9.485	152	713.578	17.351	216	1038.427	156.010
25	115.599	2.600	89	332.053	7.180	153	714.022	122.746	217	1038.697	2715.452
26	116.577	1.587	90	333.005	6.642	154	714.614	34.894	218	1052.634	158.816
27	119.183	2.251	91	336.421	32.110	155	717.285	29.890	219	1065.802	170.546
28	121.899	0.388	92	340.363	34.545	156	720.070	84.842	220	1067.788	70.227
29	122.348	0.209	93	345.475	121.678	157	726.169	75.921	221	1073.266	192.395
30	128.511	0.148	94	346.213	72.438	158	729.507	27.411	222	1077.495	350.161
31	129.693	2.309	95	350.749	198.626	159	731.735	108.571	223	1087.331	137.252
32	132.327	0.382	96	353.386	105.586	160	737.765	49.313	224	1090.453	11.936
33	136.943	0.941	97	354.859	59.466	161	741.524	13.652	225	1098.141	16.657

34	138.314	1.301	98	355.835	60.425	162	744.570	28.282	226	1101.591	198.827
35	140.109	1.524	99	357.410	43.131	163	747.744	107.820	227	1108.173	244.985
36	141.939	5.252	100	361.811	8.741	164	755.594	64.127	228	1116.342	112.437
37	152.544	2.824	101	365.012	64.435	165	771.237	6.640	229	1129.375	1889.880
38	154.374	0.563	102	368.303	45.668	166	781.317	247.544	230	1133.051	32.385
39	157.992	1.166	103	377.291	51.733	167	785.117	49.579	231	1136.967	1208.519
40	159.884	1.003	104	384.400	35.413	168	795.904	19.836	232	1142.640	1069.930
41	161.656	3.271	105	386.274	92.140	169	797.284	107.476	233	1152.482	726.988
42	167.081	0.967	106	389.759	27.273	170	800.561	105.795	234	1206.587	126.488
43	171.177	2.637	107	396.291	24.345	171	805.405	248.906	235	1731.803	114.914
44	172.767	0.186	108	404.363	8.655	172	807.433	35.829	236	1764.710	200.289
45	174.356	2.528	109	407.644	166.727	173	811.620	172.965	237	1785.776	59.953
46	177.641	2.033	110	410.106	8.781	174	814.553	60.574	238	2265.522	118.098
47	179.649	0.952	111	417.288	29.772	175	819.444	139.346	239	2301.500	71.307
48	183.487	0.470	112	426.799	5.747	176	821.815	85.475	240	2310.912	157.321
49	190.048	2.749	113	428.620	22.599	177	825.402	24.756	241	2326.252	124.021
50	192.757	30.253	114	436.060	38.786	178	832.472	183.689	242	2341.898	128.020
51	195.285	11.647	115	444.751	30.891	179	834.494	9.762	243	2356.344	101.978
52	198.500	47.363	116	449.192	220.091	180	838.882	161.833	244	3288.860	1404.348
53	204.186	13.447	117	454.436	9.298	181	850.447	144.108	245	3425.115	917.104
54	206.624	33.820	118	463.682	28.140	182	852.801	173.074	246	3470.295	350.886
55	210.542	20.338	119	468.243	24.191	183	858.929	109.339	247	3574.355	482.201
56	217.272	3.665	120	474.974	42.738	184	864.143	11.165	248	3627.762	481.512
57	226.221	9.581	121	479.904	28.635	185	866.262	59.147	249	3693.831	115.434
58	229.832	9.971	122	486.377	13.931	186	873.174	305.173	250	3723.494	102.933
59	240.005	6.086	123	498.773	40.016	187	875.636	84.470	251	3771.344	152.089
60	242.205	12.637	124	515.786	82.478	188	889.858	0.510	252	3816.668	50.220
61	246.534	5.626	125	521.062	26.405	189	894.483	0.961	253	3825.287	74.234
62	248.529	10.159	126	523.370	107.641	190	898.006	21.071	254	3855.624	102.825
63	254.208	4.657	127	533.202	26.399	191	905.468	129.982	255	3856.375	109.800
64	256.228	5.194	128	537.648	22.354	192	907.874	155.703			

Table 21

1-2H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	3.6004 eV	344.36 nm	f=0.002
Excited State 2:	Singlet-A	3.8612 eV	321.11 nm	f=0.001
Excited State 3:	Singlet-A	3.9788 eV	311.61 nm	f=0.002
Excited State 4:	Singlet-A	4.6470 eV	266.80 nm	f=0.006

2-3H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	3.3486 eV	370.26 nm	f=0.003
Excited State 2:	Singlet-A	3.4251 eV	361.98 nm	f=0.202
Excited State 3:	Singlet-A	3.4415 eV	360.26 nm	f=0.075
Excited State 4:	Singlet-A	3.9842 eV	311.19 nm	f=0.058

3-3H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	2.6046 eV	476.01 nm	f=0.006
Excited State 2:	Singlet-A	2.6332 eV	470.85 nm	f=0.146
Excited State 3:	Singlet-A	3.3730 eV	367.58 nm	f=0.002
Excited State 4:	Singlet-A	3.4166 eV	362.89 nm	f=0.260
Excited State 5:	Singlet-A	3.5656 eV	347.72 nm	f=0.001

4-4H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.6351 eV	267.49 nm	f=0.004
Excited State 2:	Singlet-A	4.8411 eV	256.11 nm	f=0.001
Excited State 3:	Singlet-A	4.9960 eV	248.17 nm	f=0.021
Excited State 4:	Singlet-A	5.0022 eV	247.86 nm	f=0.006
Excited State 5:	Singlet-A	5.0189 eV	247.04 nm	f=0.072

5-5H_2O:	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.6739 eV	265.27 nm	f=0.008
Excited State 2:	Singlet-A	4.9372 eV	251.12 nm	f=0.009

6-6H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.7318 eV	262.02 nm	f=0.003
Excited State 2:	Singlet-A	4.9319 eV	251.39 nm	f=0.001
Excited State 3:	Singlet-A	4.9456 eV	250.69 nm	f=0.009
Excited State 4:	Singlet-A	5.1352 eV	241.44 nm	f=0.040
Excited State 5:	Singlet-A	5.1466 eV	240.91 nm	f=0.003

7-1H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 9:	Singlet-A	3.2886 eV	377.02 nm	f=0.002
Excited State 10:	Singlet-A	3.3166 eV	373.83 nm	f=0.427
Excited State 12:	Singlet-A	3.5234 eV	351.89 nm	f=0.030

8-2H_2O

Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
4.7647 eV	260.21 nm	0.010
4.8126 eV	257.63 nm	0.012
4.8201 eV	257.22 nm	0.002
4.8480 eV	255.74 nm	0.001
4.8523 eV	255.52 nm	0.037

9-2H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.7680 eV	260.04 nm	f=0.010
Excited State 2:	Singlet-A	4.8126 eV	257.63 nm	f=0.011
Excited State 3:	Singlet-A	4.8210 eV	257.18 nm	f=0.003
Excited State 4:	Singlet-A	4.8520 eV	255.53 nm	f=0.014
Excited Statec 5:	Singlet-A	4.8560 eV	255.32 nm	f=0.025

10-4H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.7201 eV	262.67 nm	f=0.005
Excited State 2:	Singlet-A	4.8002 eV	258.29 nm	f=0.017
Excited State 3:	Singlet-A	4.8220 eV	257.12 nm	f=0.009
Excited State 4:	Singlet-A	4.8583 eV	255.20 nm	f=0.006
Excited State 5:	Singlet-A	4.8806 eV	254.04 nm	f=0.001
Excited State 6:	Singlet-A	4.8964 eV	253.21 nm	f=0.011

11-5H_2O:	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.6748 eV	265.22 nm	f=0.004
Excited State 2:	Singlet-A	4.7571 eV	260.63 nm	f=0.012
Excited State 3:	Singlet-A	4.8054 eV	258.01 nm	f=0.003
Excited State 4:	Singlet-A	4.8294 eV	256.73 nm	f=0.005
Excited State 5:	Singlet-A	4.8403 eV	256.15 nm	f=0.003
Excited State 6:	Singlet-A	4.8623 eV	254.99 nm	f=0.002

12-7H_2O:	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.8389 eV	256.22 nm	f=0.002
Excited State 2:	Singlet-A	4.9129 eV	252.37 nm	f=0.007
Excited State 3:	Singlet-A	4.9352 eV	251.22 nm	f=0.014
Excited State 4:	Singlet-A	4.9422 eV	250.87 nm	f=0.011
Excited State 5:	Singlet-A	4.9685 eV	249.54 nm	f=0.014

13-11H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	6.4772 eV	191.42 nm	f=0.073
Excited State 2:	Singlet-A	6.6409 eV	186.70 nm	f=0.029
Excited State 3:	Singlet-A	6.7358 eV	184.07 nm	f=0.018
Excited State 4:	Singlet-A	6.7906 eV	182.58 nm	f=0.001
Excited State 5:	Singlet-A	6.9496 eV	178.41 nm	f=0.001
Excited State 6:	Singlet-A	6.9803 eV	177.62 nm	f=0.001

14-1H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	0.4853 eV	2554.86 nm	f=0.033

15-6H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 2:	Singlet-A	3.8458 eV	322.39 nm	f=0.004

16-12H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	2.7966 eV	443.35 nm	f=0.002
Excited State 2:	Singlet-A	3.4247 eV	362.03 nm	f=0.025

18-4H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.9174 eV	252.13 nm	f=0.039
Excited State 2:	Singlet-A	4.9439 eV	250.78 nm	f=0.006
Excited State 3:	Singlet-A	4.9506 eV	250.44 nm	f=0.022
Excited State 4:	Singlet-A	4.9710 eV	249.41 nm	f=0.012
Excited State 5:	Singlet-A	4.9754 eV	249.20 nm	f=0.026
Excited State 6:	Singlet-A	4.9875 eV	248.59 nm	f=0.117

19-9H_2O	Spin & spatial symmetry	Excitation energy (eV)	Excitation energy (nm)	oscillator strengths
Excited State 1:	Singlet-A	4.8285 eV	256.78 nm	f=0.008
Excited State 2:	Singlet-A	4.8288 eV	256.76 nm	f=0.019